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Novozymes A/S

Krogshøjvej 36 DK-2880 Bagsværd

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John Nielsen

PATENT- OG VAREMÆRKESTYRELSEN

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GALACTANASE VARIANTS

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FIELD OF THE INVENTION

The present invention relates to variants of galactanases of Glycoside Hydrolase Family 53, their production, and their use within the dairy industry.

5 BACKGROUND OF THE INVENTION

Background art

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The crystallization and preliminary X-ray studies of the galactanase from *Aspergillus* aculeatus is described by Ryttersgaard et al in Acta. Cryst. (1999), D55, 929-930.

SUMMARY OF THE INVENTION

The Invention provides variants of a parent Glycoside Hydrolase Family 53 galactanase, comprising an alteration in at least one of the following positions: -6, -4, -2, 1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 18, 20, 22, 24, 25, 26, 29, 30, 31, 32, 36, 39, 40, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 54a, 54e, 54f, 54g, 54h, 55, 56, 57, 58, 61, 62, 65, 69, 77, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 101, 106, 107, 110, 113, 114, 126, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 144, 145, 146, 147, 150, 153, 157, 159, 163, 169, 171, 172, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 191, 192, 194, 198, 200, 203, 204, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234, 241, 242, 243, 244, 245, 246, 247, 248, 249, 250, 252, 252d, 252e, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 265, 266, 273, 274, 276, 277, 280, 283, 284, 286, 288, 288a, 289, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301, 302, 302a, 302d, 302j, 302k, 302m, 302n, 302o, 302q, 302r, 302s, 302t, 302u, 302v, 302x, 302y, 302z, 302aa, 302bb, 302cc, 302dd, 302ee, 302ff, 302gg, 302hh, 302ii, 302ji, 303, 304, 305, 306, 307, 308, 309, 310, 311, 312, 313, 314, 315, 316, 317, 318, 319, 320, 321, 322, 323, 324, 325, 326, 327, 328, 329, and 330; wherein

(a) the alteration(s) are independently (i) an insertion of an amino acid immediately down-stream of the position, (ii) a deletion of the amino acid which occupies the position, and/or (iii) a substitution of the amino acid which occupies the position; and (b) the variant has galactanase activity.

BRIEF DESCRIPTION OF DRAWINGS

Fig. 1 shows the coordinates for the 3D structure of a GH Family 53 galactanase from *Myceliophthora thermophila* having SEQ ID NO: 1;

Fig. 2 shows the coordinates for the 3D structure of a GH Family 53 galactanase from Humicola insolens having SEQ ID NO: 2;

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Fig. 3 shows the coordinates for the 3D structure of a GH Family 53 galactanase from Aspergillus aculeatus having SEQ ID NO: 3;

Fig. 4 shows the coordinates for the 3D structure of a GH Family 53 galactanase from *Bacillus licheniformis* having SEQ ID NO: 4;

Fig. 5 shows a multiple alignment of SEQ ID NOs: 1-4; and

Fig. 6 shows the alignment of Fig. 5 with three additional galactanase sequences added.

DETAILED DESCRIPTION OF THE INVENTION

3D-structure determination

The crystallization and preliminary X-ray studies of the galactanase from Aspergillus aculeatus (AAGAL) is described by Ryttersgaard et al in Acta. Cryst. (1999), D55, 929-930. The galactanases from Myceliophthora thermophila (MTGAL) and Humicola insolens (HIGAL) (WO 97/32014), and the galactanase from Bacillus licheniformis (BLGAL) (WO 00/47711) were crystallized using similar principles.

The 3D-structures were solved in accordance with the principles for X-ray crystallographic methods as given, for example, in X-Ray Structure Determination, Stout, G.K. and Jensen, L.H., John Wiley & Sons, Inc. NY, 1989. The structural coordinates for the crystal structure of the *Aspergillus aculeatus* galactanase (AAGAL), as determined by multiple isomorphous replacement to 1.8 Å resolution at 100 K are given in Fig. 1 in standard PDB format (Protein Data Bank, Brookhaven National Laboratory, Brookhaven, CT).

The structures of the other three galactanases were solved by Molecular Replacement, using the AAGAL293 structure (to 2.3 Å resolution at 293K) as a search model. Data from 20-2.55 Å, 18-2.14 Å, and 19.67-2.60 Å were used for HIGAL, MTGAL and BLGAL, respectively, within AMoRe (J. Navaza: AMoRe: an Automated package for Molecular Replacement. Acta Crystallogr., A50:157-163, 1994). The respective coordinates are given in Figs. 2-4 in standard PDB format.

Variant

The term "galactanase variant," or simply "variant," refers to a galactanase comprising one or more alteration(s), such as substitution(s), insertion(s), deletion(s), and/or truncation(s) of one or more specific amino acid residue(s) in one or more specific position(s) in a parent galactanase.

The total number of such alterations is typically not more than thirty, e.g. one, two, three, four, five, six, seven, eight, nine, ten, eleven, twelve, thirteen, fourteen, fifteen, sixteen, seventeen, eighteen, nineteen, twenty, twenty-one, twenty-two, twenty-three, twenty-four, twenty-five, twenty-six, twenty-seven, twenty-eight, twenty-nine, or thirty of said alterations.

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In addition, the variant of the invention may include other modifications of the parent enzyme, typically not more than 10, e.g. not more than 5 such modifications.

Nomenclature and conventions for designation of variants

A substitution in a variant is indicated as "original amino acid - position - substituted amino acid." The one letter code is preferably used, but it can of course be translated into the three letter code as desired. The codes X (or Xaa) may be used to indicate any amino acid residue. Accordingly, the notation "D182N" or means, that the variant comprises a substitution of aspartic acid with asparagine acid in the variant amino acid position corresponding to the amino acid in position 182 in MTGAL, when the two are aligned as indicated in Fig. 5.

Where the original amino acid residue may be any amino acid residue, a short hand notation may at times be used indicating only the position, and the substituted amino acid, for example: "Position - substituted amino acid", or "182N". This notation is particular relevant in connection with modification(s) in a series of homologous polypeptides, such as the galactanases of GH Family 53. Similarly when the identity of the substituting amino acid residue(s) is immaterial: "Original amino acid - position;" or "D182".

When both the original amino acid(s) and substituted amino acid(s) may be any amino acid, then only the position is indicated, e.g. "182".

When the original amino acid(s) and/or substituted amino acid(s) may comprise more than one, but not all amino acid(s), then the amino acids are listed, separated by commas: "Original amino acid - position no. - substituted amino acid"; e.g. "H91D,L,N".

A number of examples of this nomenclature are listed below:

The substitution of aspartic acid for asparagine in position 182 is designated as D182N.

The substitution of any amino acid residue for serine in position 131 is designated as S131X, or S131.

The substitution of proline for any amino acid residue in position 29 would thus be designated X29P, or 29P.

For a modification where the original amino acid(s) and/or substituted amino acid(s) may comprise more than one, but not all amino acid(s), the substitution of aspartic acid, leucine, or asparagine for histidine in position 91 would be indicated by H91D,L,N; which indicates the specific variants H91D, H91L, or H91N.

A deletion of glutamic acid in position 288a will be indicated by E288a*. Correspondingly, the deletion of more than one amino acid residue, such as the deletion of glutamic acid and aspartic acid in positions 252a and 252b will be designated"E252a*+D252b*"

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A truncation means an N- or C-terminal shortening of the complete amino acid sequence, i.e. a deletion of one, or usually more, amino acids and the N- or C-terminal end of the peptide. As regards the designation of truncated variants, the general rule for deletions may be used.

The insertion of an additional amino acid residue such as e.g. a valine after F216 is indicated by "F216FV"; or, when more than one amino acid residue is inserted, such as e.g. a valine, alanlne, serine, threonine and a glycine after F216 this will be indicated as: "F216FVASTG".

In such cases the inserted amino acid residue(s) are numbered by the addition of lower case letters to the position number of the amino acid residue preceding the inserted amino acid residue(s). In the above example the sequences would thus be:

Parent: Variant:
216 216 216a 216b 216c 216d 216e 217
F F V A S T G Y

Once all lower case letters from a to z (a,b,c,d,e,f,g,h,i,j,k,l,m,n,o,p,q,r,s,t,u,v,x,y,z) have been used for this purpose, double letters aa, bb, cc etc. onto zz are used, see e.g. the alignment of Fig. 5, between positions 302 and 303.

In cases where an amino acid residue identical to the existing amino acid residue is inserted, it is clear that degeneracy in the nomenclature arises. If for example a phenylalanine would be inserted after the phenylalanine in the above example this would be indicated by "F216FF".

Given that a proline is present in position 215, the same actual change could just as well be indicated as "P215PF":

Parent: Variant: Numbering I: 215 216 215 216 216a Sequence: Ρ F P F F Numbering II: 215 215a 216

Such instances will be apparent to the skilled person, and the indication "F216FF" and corresponding indications for this type of insertions is thus meant to comprise such equivalent degenerate indications.

By analogy, if amino acid sequence segments are repeated in the parent galactanase and/or in the variant, it will be apparent to the skilled person that equivalent degenerate indications are comprised, also when other alterations than insertions are listed such as deletions and/or substitutions. For instance, the deletion of two consecutive amino acids "DG" in the sequence "DGDG" from position 252b-252e, may be written as "D252b*+G252c*" or "D252d*+G252e*" or "G252c*+D252d*":

Parent: Variant: Numbering I: 252b 252c 252d 252e 252b 252c

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 Sequence:
 D
 G
 D
 G

 Numbering II:
 252d
 252e

 Numbering III:
 252b
 252e

Variants comprising multiple modifications are separated by pluses, e.g. "A90S+H91D"

representing modifications in positions 90 and 91 substituting tyrosine and glutamic acid for arginine and glycine, respectively. Thus, "A90S+H91D,N,L" designates the following variants: A90S+H91D, A90S+H91N, and A90S+H91L. Likewise, N303D,H+N305D,H,P designates the following variants: N303D+N305D; N303D+N305H; N303D+N305P; N303H+N305D; N303H+N305H, and N303H+N305P.

This nomenclature is particular relevant relating to modifications aimed at substituting, inserting or deleting amino acid residues having specific common properties, such modifications are referred to as conservative amino acid modification(s). Examples of conservative modifications are within the group of basic amino acids (arginine, lysine and histidine), acidic amino acids (glutamic acid and aspartic acid), polar amino acids (glutamine and asparagine), hydrophobic amino acids (leucine, isoleucine and valine), aromatic amino acids (phenylalanine, tryptophan and tyrosine), and small amino acids (glycine, alanine, serine, threonine and methionine). Amino acid modifications, which do not generally alter the specific activity are known in the art and are described, for example, by H. Neurath and R.L. Hill, 1979, In, The Proteins, Academic Press, New York. The most commonly occurring exchanges are Ala/Ser, Val/Ile, Asp/Glu, Thr/Ser, Ala/Gly, Ala/Thr, Ser/Asn, Ala/Val, Ser/Gly, Tyr/Phe, Ala/Pro, Lys/Arg, Asp/Asn, Leu/Ile, Leu/Val, Ala/Glu, and Asp/Gly as well as the in reverse.

For the present purposes, the sequence of MTGAL (SEQ ID NO:1) has been selected as the frame of reference, meaning that all variants will be defined on the basis of the amino acid sequence of MTGAL. In particular, each amino acid residue in a galactanase sequence is assigned a number, a position, or a position number, by reference to Fig. 5 herein, viz. the number of the corresponding amino acid residue in the *Myceliophthora thermophila* galactanase backbone (MT; the uppermost line of the alignment of Fig. 5). In this context, the term "corresponding" refers to the amino acid which, according to the alignment, is in the same column as the amino acid residue in question, but in the first row designated "MT".

For example, the variant of the galactanase from *Bacillus licheniformis* (BL) which by reference to SEQ ID NO: 4 may be designated S39C will, for the present purposes, be designated S18C, because S39 of BL corresponds to A18 of MT. As another example, the variant of the galactanase from *Aspergillus aculeatus* which by reference to SEQ ID NO: 3 may be designated D182N will, for the present purposes, be designated D181N, because D182 of AA corresponds to N181 of MT. As a still further example, variant K16P of BL may

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be designated *-6P, because K16P of BL corresponds to a missing or deleted amino acid in position -6 of MT, still by strict formal reference to Fig. 5.

However, if desired, the variants of the invention may also be defined by reference to their respective "own" backbone, e.g. with reference to SEQ ID NO:1, SEQ ID NO:2, SEQ ID NO: 3, or SEQ ID NO: 4. The corresponding position numbers are easily deduced, in the same way as described above, from Figs. 5-6 or, for additional galactanase sequences, from a figure which can be prepared according to the principles described herein.

Molecular Dynamics (MD)

Molecular Dynamics (MD) simulations are indicative of the mobility of the amino acids in a protein structure (see McCammon, JA and Harvey, SC., (1987), "Dynamics of proteins and nucleic acids", Cambridge University Press). Such protein dynamics are often compared to the crystallographic B-factors (see Stout, GH and Jensen, LH, (1989), "X-ray structure determination", Wiley). By running the MD simulation at, e.g., different temperatures, the temperature related mobility of residues is simulated. Regions having the highest mobility or flexibility (here isotropic fluctuations) may be suggested for random mutagenesis. It is here understood that the high mobility found in certain areas of the protein, may be thermally improved by substituting these residues.

Variants of amended properties

Based on the 3D-structure of the galactanase from *Myceliophthora thermophila* of SEQ ID NO:1, the following variants are contemplated, in which at least one of the below-mentioned residues have been amended and/or at least one of the below-mentioned alterations have been introduced:

i) variants of an amended specific activity, within 10Å from the active site: Y4, G6, V7, D8, W9, S10, R45, Q46, R47, W49, Y77, D79, F80, H81, Y82, W86, A87, D88, P89, A90, H91, Q92, T93, S131, I132, G133, N134, E135, I136, R137, A138, G139, L140, L141, W142, G145, R146, T147, I153, L157, M176, I177, H178, L179, D180, N181, G182, W183, T187, Q188, W191, Y192, M209, G210, V211, S212, F213, Y214, P215, F216, Y217, A221, L226, I241, A242, V243, V244, E245, T246, N247, W248, F276, I277, V280, V284, G292, L293, F294, Y295, W296, E297, P298, W300, L306, G307, F329;

ii) variants of an amended activity on lactose, within 10Å from the active site: Y214S,N+N247Y+L306Q; Y214A; F216FVASTGY217; P89W+W86N;

iii) variants of an amended pH-activity profile: H91N,L,D; N313D; N303D,H; N305D,H; A90S+H91D;

iv) variants of an amended thermostability, by insertion of prolines: Y22P, N24P, T25P, A29P, A53P, N56P, T93P, D101P, W142P, T147P, Q198P, L203P, S204P, S219P, S258P, S288P, A304P, A311P, Q318P, A322P, S324P, S325P, S327P;

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- v) variants of an amended thermostability, by increasing surface hydrophobicity: W107S,H;
- vi) variants of an amended thermostability, by amending the surface electrostatic potential: Q126E;
- vii) variants of an amended thermostability, by disulfide bridges (double mutations to cysteines): V20C+G320C, N39C+L326C, Y110C+G163C, W150C+N194C, T274C+V328C, V301C+F316C
- viii) variants of amended thermostability, by improved side-chain packing: 18F,Y,W; 12V, 80F, 82Y, 191Y,W; 213F; 18W+12V; 80F+82Y.

Based on the 3D-structure of the galactanase from *Humicola insolens*, the following variants are contemplated, in which at least one of the below-mentioned residues have been amended and/or at least one of the below-mentioned alterations have been introduced:

- i) variants of an amended thermostability, by insertion of prolines: V20P, V25P, E29P, V41P, V50P, W53P, N56P, T94P, A96P, W142P, L169P, W185P, Q198P, M203P, A219P, A221P, T222P, Q258P, A261P, D262P, S288P, N305P, A311P, A322P, S324P, S325P.
- ii) variants of an amended thermostability, by disulfide bridges (double mutations to cysteines): T113C+G163C, W185C+S229C, S218C+A221C, R227C+V283C.

Based on the 3D-structure of the galactanase from Aspergillus aculeatus, the following variants are contemplated, in which at least one of the below-mentioned residues have been amended and/or at least one of the below-mentioned alterations have been introduced::

- i) variants of an amended pH-activity profile: D181N;
- ii) variants of an amended thermostability, by Insertion of prolines: T3P, Y20P, N24P, L25P, T29P, A31P, V50P, S53P, S56P, T93P, T94P, S96P, W142P, L144P, E146P, T147P, T172P, E200P, S203P, A219P, A256P, A258P, S261P, S264P, I266P, T288P, I301P, A304P, Y318P, E324P;
- iii) variants of an amended thermostability, by disulfide bridges (double mutations to cysteines): L13C+L65C, N24C+Q30C, S218C+A221C, A304C+Y318C.

Based on the 3D-structure of the galactanase from *Bacillus licheniformis*, the following variants are contemplated, in which at least one of the below-mentioned residues have been amended and/or at least one of the below-mentioned alterations have been introduced::

- i) variants of an amended thermostability, by insertion of prolines: K-6P, S-4P, L-2P, K1P, V20P, S26P, K29P, D31P, A54aP, G54eP, N57P, K93P, A97P, N101P, S171P, S185P, T256P, N260P, N266P, D286P, E288aP, A289P, A302dP, S302yP, Y302zP, A302bP, E302ccP, E302ggP, F305P, D311P, F318P;
- ii) variants of an amended thermostability, by disulfide bridges (double mutations to cysteines): S18C+Y302qC, G40C+Q330C, V44C+A69C, I48C+A62C, N50C+D84C,

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G54gC+T302xC, N56C+G302rC, A62C+G146C, K106C+A159C, K114C+A163C, E183C+G221C, T227C+A283C, A234C+V241C, Y250C+Q273C, A302aaC+A302iiC.

Additional variants of the Invention which may exhibit amended properties as regards substrate binding and/or substrate specificity are listed below.

According to "Nomenclature for sugar-binding subsites in glycosyl hydrolases", G.J. Davis, K.S. Wilson and B. Henrissart, Biochemical Journal, Volume 321, pages 557 to 559 (1997), so-called subsites may be determined. Such subsites may be labelled from -N to +N (where N is an integer). -N represents the non reducing end and +N the reducing end of the polysaccharide. The cleaveage is taking place between the -1 and +1 subsites. The principal constituent of a sugar binding subsite is also called an aromatic platform. That is an aromatic residue, i.e. one of the following: W, H, Y or F.

Based on Figs. 1-4 the inventors identified subsites as follows:

For MTGAL, HIGAI and AAGAL the following subsites were identified, reference being here had to the position numbering of SEQ ID NOs 1, 2, and 3, respectively (not to the corresponding residue in SEQ ID NO: 1):

Subsite -4: MTGAL none; HIGAL W53; AAGAL none.

Subsite -2: MTGAL W86, W300; HIGAL W86, W300; AAGAL W86, W301.

Subsite -1: MTGAL W296; HIGAL W296; AAGAL W297.

Subsite +1: MTGAL Y217, Y214; HIGAL Y217, Y214; AAGAL Y218, Y215.

20 Subsite +2: MT W183; HIGAL W183; AAGAL W184.

For BLGAL the following subsites were identified, reference being here had to the position numbering of SEQ ID NO: 4 (not to the corresponding residue in SEQ ID NO: 1):

Subsite -4: W363.

Subsite -3: W347.

25 Subsite -2: W115.

Subsite -1: W320.

Subsite +1: W237, Y234.

Also the residues in the near vicinity (5 Å) of the above residues may be altered and provide an amended substrate specificity and/or substrate binding. These residues are the following, reference being here had to the position numbering of SEQ ID NOs 1, 2, 3, and 4, respectively (not to the corresponding residue in SEQ ID NO: 1):

MTGAL (SEQ ID NO: 1): G6, V7, D8, W9, S10, S11, V12, V13, V14, E15, E16, A18, V20, Y22, L32, L36, T43, V44, R45, Q46, R47, V48, W49, V50, N51, P52, D54, N56, Y57, Y61, Y77, D79, F80, H81, Y82, S83, D84, T85, W86, A87, D88, P89, A90, H91, Q92, T93, M94, P95, G133, N134, E135, I136, R137, G139, L140, L141, W142, H178, L179, D180, N181, G182, W183, D184, W185, G186, T187, Q188, N189, G210, V211, S212, F213, Y214, P215, F216, Y217, S218, S219, S220, A221, T222, L223, S224, A225, L226, K227, S228, S229, L230, D231, N232, M233, I241, A242, V243, V244, E245, T246, N247, W248,

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P249, I250, C252, P255, R256, Y257, S258, F259, P260, D262, V263, Q273, F276, I277, V280, I283, L293, F294, Y295, W296, E297, P298, A299, W300, I301, H302, N303, A304, N305, L306, G307, S308, S309, C310, A311, D312, N313, T314, M315, F316, S317, Q318, S319, G320, Q321, L326, F329.

HIGAL (SEQ ID NO: 2): G6, V7, D8, W9, S10, S11, V12, M13, V14, E15, E16, A18, V20, Y22, L32, L36, M43, V44, R45, Q46, R47, V48, W49, V50, N51, P52, W53, D54, G55, N56, Y57, N58, Y61, Y77, N79, F80, H81, Y82, S83, D84, T85, W86, A87, D88, P89, A90, H91, Q92, T93, T94, A96, G133, N134, E135, I136, T137, G139, L141, W142, H178, L179, D180, N181, G182, W183, N184, W185, D186, T187, Q188, N189, G210, V211, S212, F213,

Y214, P215, F216, Y217, S218, A219, S220, A221, T222, L223, D224, S225, L226, R227, R228, S229, L230, N231, N232, M233, V241, A242, V243, V244, E245, T246, N247, W248, P249, C252, P255, R256, Y257, Q258, F259, P260, D262, V263, Q273, Y276, I277, V280, V283, L293, F294, Y295, W296, E297, P298, A299, W300, I301, H302, N303, A304, N305, L306, G307, S308, S309, C310, A311, D312, N313, T314, M315, F316, T317, P318, S319, G320, Q321, L326, F329.

AAGAL (SEQ ID NO: 3): R5, G6, A7, D8, I9, S10, S11, L12, L13, L14, L15, E16, E18, Y20, Y22, L32, L36, S43, I44, R45, Q46, R47, V48, W49, V50, N51, P52, D54, S56, Y57, Y61, Y77, D79, L80, H81, L82, S83, D84, T85, W86, A87, D88, P89, S90, D91, Q92, T93, T94, P95, G134, N135, E136, I137, R138, G140, L142, W143, H179, L180, D181, D182, G183, W184, S185, W186, D187, Q188, Q189, N190, G211, V212, S213, Y214, Y215, P216, F217, Y218, S219, A220, S221, A222, T223, L224, A225, S226, L227, K228, T229, S230, L231, A232, N233, L234, V243, V244, V245, E246, T247, N248, W249, P250, C253, P256, A257, Y258, A259, F260, P261, D263, L264, Q274, F277, L278, L281, V284, V294, Y295, Y296, W297, E298, P299, A300, W301, I302, G303, N304, A305, G306, L307, G308, S309, S310, C311, A312, D313, N314, L315, M316, V317, D318, Y319, T320, D322, V324, Y325, I328, L331.

BLGAL (SEQ ID NO: 4): K26, G27, V28, D29, V30, S31, S32, A35, L36, Y64, V65, R66, V67, R68, I69, W70, N71, D72, P73, Y74, G80, Y81, G82, G83, G84, N85, N86, L106, D108, F109, H110, Y111, S112, D113, F114, W115, A116, D117, P118, A119, K120, Q121, K122, A123, P124, Q161, G163, N164, E165, T166, G169, A171, G172, H202, F203, T204, N205, P206, E207, T208, R211, Y212, S231, S232, Y233, Y234, P235, F236, W237, H238, G239, T240, L241, N243, L244, V261, A262, E263, T264, S265, Y266, T267, D274, G275, H276, G277, N278, T279, A280, P281, K282, N283, G284, Q285, T286, L287, N288, Q296, A299, V300, V303, V317, F318, Y319, W320, E321, P322, A323, W324, I325, V327, N336, K337, L339, W340, E341, Y343, G344, S345, G346, W347, A348, T349, S350, Y351, A352, A353, Y355, D356, P357, E358, D359, A360, G361, K362, W363, F364, G365, G366, S367, A368, V369, D370, N371, Q372, A373, L374, F375, F388.

The above amino acids may be substituted with any other amino acid, e.g. any of the remaining 19 natural amino acids. In the variants of the invention, at least one of the above-mentioned residues have been amended to introduce either of the other nineteen amino acid residues. The above variants are also included in dependent claims, however in the claims they have been renumbered according to the principles outlined above, each position being assigned the number of the corresponding amino acid residue in SEQ ID NO: 1.

<u>Alignments</u>

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The program ClustalW (CLUSTAL W: improving the sensitivity of progressive multiple sequence alignment through sequence weighting, position specific gap penalties and weight matrix choice." Julie D. Thompson, Desmond G. Higgins, and Toby J. Gibson, Nucleic Acids Research, 22(22):4673-4680 (1994)) is used for the purposes of the present invention for pairwise protein sequence alignments, multiple protein sequence alignments and protein profile alignments (version 1.82, default parameters).

For pairwise sequence comparison and calculation of percentage identity, the pairwise alignment parameters were: Slow/Accurate; Gap Open Penalty=10.00; Gap Extension Penalty=0.10; Protein weight matrix=Gonnet series; DNA weight matrix=IUB.

The consensus length is calculated automatically by the program. The number of identical residues (identified with an asterisk) is counted. The percentage of sequence identity is calculated as follows: the number of identical residues is divided by the consensus length and multiplied by 100.

The multiple alignment of Fig. 5 is based on a multiple alignment of the four sequences using Clustalw, but, importantly, it is combined with information derived from the 3D-structures, each position in each backbone being carefully evaluated, and the alignment modified by the present inventors. In other words, the multiple alignment of Fig. 5 is not a simple ClustalW multiple alignment reflecting only sequence homologies, it also reflects structural similarities.

The alignment of Fig. 5 can therefore be used to deduce corresponding variants in other backbones, and these variants are likely to also exhibit the amended property in question. For example, the above-mentioned variant A90S+H91D of MT is transferable to the other backbones or parent galactanases shown in Fig. 5 as follows: According to the Fig. 5 alignment, this variant would correspond to: A90S+H91D of HI; and A90S+K91D of BL. Because AA already has the sequence of S90D91, this variant is not relevant for AA. Another example is variant T288P of AA, which, using the alignment of Fig. 5, translates into S288P in MT and HI, and G288P in BL.

Other galactanase backbones of Glycoside Family 53 are known (see below under parents), and these can be added to the alignment of Fig. 5 as described below, and thereby corresponding variants can be deduced also for these backbones, as just described above.

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For aligning a new sequence to the multiple alignment of Fig. 5, the Clustalw option called profile alignment is used as follows: The Fig. 5 multiple alignment is used as profile 1, and then the new sequence as profile 2. Then the program is asked to "Align sequence to 1st. profile," using the following parameters:

Multiple alignment parameters = Slow/Accurate; Gap Open Penalty=10.00; Gap Extension Penalty=0.20; Delay divergent sequences=30%; DNA Transitions Weight:0.50; Protein weight matrix=Gonnet series; DNA weight matrix=IUB; Use negative matrix=OFF;

Protein Gap Parameters: Toggle Residue-Specific Penalties=ON; Toggle Hydrophilic Penalties=ON; Hydrophilic Residues= GPSNDQEKR; Gap Separation Distance =4; Toggle End Gap Separation=OFF.

In Fig. 6, as an example, three new galactanase sequences have been added to the Fig. 5 alignment. The new galactanases are added at the bottom of the alignment, as rows nos. 5, 6 and 7. The galactanases are: AT (the galactanase of *Aspergillus tubigensis*, (SEQ ID NO: 7)); BS (the galactanase of *Bacillus subtilis* (SEQ ID NO: 8)); and PF (the galactanase of *Pseudomonas fluorescens* (SEQ ID NO: 9)). Thus, using Fig. 6, the abovementioned variant A90S+H91D of MT translates into A90S+K91D of BS, and E90S+K91D of PF. Because AT already has the sequence of S90D91, this variant is not relevant for AT. Another example is variant T288P of AA, which, using the alignment of Fig. 6, translates into variants T288P of AT, G288P of BS, and G288P of PF.

In the alternative, alignments of sequences and calculation of degree %-identity may be done using a full Smith-Waterman alignment, useful for both protein and DNA alignments. The default scoring matrices BLOSUM50 and the identity matrix are used for protein and DNA alignments respectively. The penalty for the first residue in a gap is -12 for proteins and -16 for DNA, while the penalty for additional residues in a gap is -2 for proteins and -4 for DNA. Alignment may be made with the FASTA package version v20u6 (W. R. Pearson and D. J. Lipman (1988), "Improved Tools for Biological Sequence Analysis", PNAS 85:2444-2448, and W. R. Pearson (1990) "Rapid and Sensitive Sequence Comparison with FASTP and FASTA", Methods in Enzymology, 183:63-98),

<u>Parent</u>

The term "parent galactanase," or simply "parent," refers to the galactanase on which the variant was based, and also to the galactanase with which the variant is compared and aligned.

The parent may be a naturally occurring (wildtype) galactanase, or it may in turn even be a variant thereof, prepared by any suitable means. For instance, the parent galactanase may be a variant of a naturally occurring galactanase which has been modified or altered in the amino acid sequence. A parent may also be an allelic variant which is any of two or more alternative forms of a gene occupying the same chromosomal locus. Allelic variation arises

naturally through mutation, and may result in polymorphism within populations as is well-described in the art. An allelic variant of a polypeptide is a polypeptide encoded by the corresponding allelic variant of a gene.

5 Galactanase

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This section is applicable to the parent galactanases, as well as the variant galactanases of the invention.

Galactanases catalyze the endohydrolysis of 1,4-beta-D-galactosidic linkages in arabinogalactans of type I and/or galactans (see the structure of rhamnogalacturonan I as described in Carpita et al. in Plant J.; 3:1-30, 1993).

In the present context, a galactanase is a polypeptide having galactanase activity. Galactanase activity can be measured using a substrate including 1,4-beta-D-galactosidic linkages. Examples of galactanase substrates are arabinogalactans of type I and galactans. Particularly suitable substrates are i) lupin galactan, and potato galactan (commercially available from, e.g., MegaZyme, Australia); as well as ii) AZCL-galactan substrates such as AZCL-potato-galactan, and AZCL-lupin-galactan (also commercially available from MegaZyme, Australia). For the substrates mentioned under i) above, galactanase activity may be measured as release of reducing sugars, whereas for the AZCL-substrates, the galactanase activity is measured spectrophotometrically (formation of a blue colour). In a particular embodiment, the galactanase assay is based on the substrate lupin AZCL galactan.

The person skilled in the art will know how to adapt assay-pH and assay-temperature to the galactanase in question. Examples of assay-pH-values are pH 2, 3, 4, 5, 6, 7, 8, 9, 10, or 11. Examples of assay-temperatures are 20, 25, 30, 35, 37, 40, 45, 50, 55, 60, 65, 70, 75, 80, or 90°C.

A preferred galactanase assay is described in Example 2 herein.

In a particular embodiment, the galactanase is an enzyme classified as ÉC 3.2.1.89, the official name of which is arabinogalactan-endo-1,4-beta-galactosidase. Alternative names are endo-1,4-beta-galactanase, galactanase, or arabinogalactanase. EC refers to Enzyme Class as described at a) http://www.chem.qmul.ac.uk/iubmb/enzyme/, and/or in b) Enzyme Nomenclature 1992 from NC-IUBMB, Academic Press, San Diego, California, published by Academic Press for IUBMB in 1992 (ISBN 0-12-227164-5), as regularly supplemented and updated. For supplements and updates, please consult

http://www.chem.gmul.ac.uk/iubmb/enzyme/supplements/, giving details regarding the following supplements: Supplement 1 (1993) (Eur. J. Biochem., 1994 223, 1-5); Supplement 2 (1994) (Eur. J. Biochem., 1995 232, 1-6); Supplement 3 (1995) (Eur. J. Biochem., 1996 237, 1-5); Supplement 4 (1997) (Eur. J. Biochem., 1997, 250, 1-6); Supplement 5 (1999)

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(Eur. J. Biochem., 1999, 264, 610-650): Supplement 6 (2000); Supplement 7 (2001); and Supplement 8 (2002).

Glycoside Hydrolase (GH) Family 53

The EC-classification referred to above is mainly based on substrate specificity of the enzymes, and does therefore not reflect the structural features of these enzymes. A classification of glycoside hydrolases in families based on amino acid sequence similarities has been proposed a few years ago; see the CAZy(ModO) site at the internet:

Coutinho, P.M. & Henrissat, B. (1999) Carbohydrate-Active Enzymes server at URL: http://afmb.cnrs-mrs.fr/~cazy/CAZY/index.html; and/or Coutinho, P.M. & Henrissat, B. (1999) Carbohydrate-active enzymes: an integrated database approach. In "Recent Advances in Carbohydrate Bioengineering", H.J. Gilbert, G. Davies, B. Henrissat and B. Svensson eds., The Royal Society of Chemistry, Cambridge, pp. 3-12; Coutinho, P.M. & Henrissat, B. (1999) The modular structure of cellulases and other carbohydrate-active enzymes: an integrated database approach. In "Genetics, Biochemistry and Ecology of Cellulose Degradation"., K. Ohmiya, K. Hayashi, K. Sakka, Y. Kobayashi, S. Karita and T. Kimura eds., Uni Publishers Co., Tokyo, pp. 15-23; Henrissat B., A classification of glycosyl hydrolases based on amino-acid sequence similarities. Biochem. J. 280:309-316(1991); Henrissat B., Bairoch A. New families in the classification of glycosyl hydrolases based on amino-acid sequence similarities. Biochem. J. 293:781-788(1993); Henrissat B., Bairoch A. Updating the sequence-based classification of glycosyl hydrolases. Biochem. J. 316:695-696(1996); and/or Davies G., Henrissat B. Structures and mechanisms of glycosyl hydrolases. Structure 3:853-859(1995).

Glycoside Hydrolase Family 53 is found under the entry relating to Glycosidases and Transglycosidases (or Glycoside Hydrolases).

These are particular embodiments of the GH Family 53 galactanase,

- i) it is an endo-1,4-beta-galactanase (EC 3.2.1.89);
- ii) it has a retaining catalytic mechanism;
- iii) it has Glu as a catalytic nucleophile or base;
- iv) it has Glu as a catalytic proton donor;
- v) its 3D Structure has a fold (beta/alpha)₆; and/or
- vi) it belongs to GH Clan GH-A.

For the purposes of the present invention, the below glycoside hydrolases of Family 53 are non-limiting examples of a parent galactanase:

Protein	Organism	GenBank	GenPept	SwissProt	Publication
naiactanaco	Aspergillus aculeatus	L34599	AAA32692.1		Christgau et al, Curr. Ge- net. 27:135-

					141(1995)
endo-1,4- beta- galactanase (GalA)	Aspergillus niger	AJ305303	CAC83735.1	Q8X168	-
galactanase GalA	Aspergillus tubin- gensis	AJ012316	CAB40555.1	Q9Y7F8	Van der Vlugt- Bergmans et al, Biotechnol. Tech. 13:87- 92(1999)
ORF 1	Bacillus circulans	L03425	AAA22259.1	P48843	SEQ ID NO:10 of WO 00/47711
ORF BH2023	Bacillus halodurans	AP001514 NC_002570	BAB05742.1 NP_242889.1	Q9KBA5	Takami et al, Extremophiles 3 (1), 21-28 (1999)
ORF yvfO	Bacillus subtilis	Z94043 Z99121	CAB08009.1- CAB15417.1	O07013 O07013 O32260	SEQ ID NO: 14 of WO 00/47711
YvfO	Bifidobacterium Iongum	AE014643 NC_004307	AAN24099.1 NP_695463.1		Schell et al, Proc. Natl. Acad. Sci. U.S.A. 99 (22), 14422- 14427 (2002)
galactanase	cus	X91885	CAA62990.1	P48841	Braithwaite et al, Biochemis- try 36:15489- 15500 (1997)
ORF CAC2570	Clostridium ace- tobutylicum	AE007755	AAK80519.1	Q97G04	Nolling et al, J. Bacteriol, 183 (16), 4823- 4838 (2001)
ORF TM1201	Thermotoga mari- tima	AE001777 NC_000853	AAD36276.1 NP_229006.1	Q9X0S8	Nelson et al, Nature 399:323- 329(1999)
	Myceliophthora thermophila	AAE73520	AAE73520.1		US 6242237
Sequence 4 from patent US 6242237	Humicola inso- lens	AAE73521	AAE73521.1		US 6242237
ORF GalA	Xanthomonas axonopodis pv.	AE011762 NC_003919	AAM36180.1 NP_641644.1		da Silva et al, Nature 417 (6887), 459-

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	citri			<u> </u>	463 (2002)
ORF XAC0575	Xanthomonas axonopodis pv. citri	AE011684 NC_003919	AAM35464.1 NP_640928.1		da Silva et al, Nature 417 (6887), 459- 463 (2002)
ORF GalA	Xanthomonas campestris pv. campestris	AE012224 NC_003902	AAM40555.1 NP_636631.1		da Silva et al, Nature 417 (6887), 459- 463 (2002)
ORF GalA	Xanthomonas campestris pv. campestris	AE012483 NC_003902	AAM42894.1 NP_638970.1		da Silva et al, Nature 417 (6887), 459- 463 (2002)
ORF YPO0853	Yersinia pestis	AJ414145 NC_003143	CAC89700.1 NP_404474.1	Q8ZHN7	Parkhill et al, Nature 413:523- 527(2001)
ORF Y3238	Yersinia pestis	AE013925 NC_004088	AAM86788.1 NP_670537.1		Deng et al J. Bacteriol. 184 (16), 4601- 4611 (2002)

Additional examples of a parent galactanase of the invention are the galactanases derived from *Meripilus giganteus* (SEQ ID NO: 2 of WO 97/32013), *Pseudomonas fluorescens*, *Bacillus agaradhaerens* (SEQ ID NO: 12 of WO 00/47711), and *Bacillus licheniformis* (SEQ ID NO: 8 of WO 00/47711).

The present invention specifically includes variants of each and every of the above specific parent galactanases of GH Family 53 corresponding to the claimed variants of MTGAL, HIGAL, AAGAL and BLGAL, such variants being derivable by adding the parent galactanase sequence in question to the Fig. 5 alignment as described above for the construction of Fig. 6, and translating each MTGAL, HIGAL, AAGAL, or BLGAL variant into the parent galactanase in question, using the concept of corresponding amino acid residue as defined above.

In a first embodiment, the parent GH Family 53 galactanase is a fungal galactanase. The fungal galactanase may be derived from a yeast, or from a filamentous fungus. The yeast galactanase may be derived from Yersinia, e.g. from Yersinia pestis. The filamentous fungal galactanase may be derived from a strain of Aspergillus, Humicola, Meripilus, Myceliophthora, or Thermomyces. Examples of these strains are Aspergillus aculeatus, Aspergillus niger, Aspergillus tubingensis, Humicola insolens, Meripilus giganteus, and Myceliophthora thermophila.

In a second embodiment, the parent GH Family 53 galactanase is a bacterial galactanase. The bacterial galactanase may be derived from a strain of Bacillus, Bifidobacterium, Cellvibrio, Clostridium, Pseudomonas, Thermotoga, or Xanthomonas.

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Examples of such strains are Bacillus agaradhaerens, Bacillus circulans, Bacillus halodurans, Bacillus licheniformis, Bacillus subtilis, Bifidobacterium longum, Cellvibrio japonicus, Clostridium acetobutylicum, Pseudomonas fluorescens, Pseudomonas cellulosa, Thermotoga maritime, Xanthomonas axonopodis pv. citri, and Xanthomonas campestris pv. campestris.

Particularly preferred parent galactanases are those with the above-mentioned GenBank, GenPept, or SwissProt accession numbers, and those with the above-mentioned SEQ ID NO's.

Further particularly preferred GH Family 53 parent galactanases are the following:

Strain of origin	Sequence Number (herein)	Abbreviations used herein
Myceliophthora thermophila	SEQ ID NO: 1	MTGAL, or MT
Humicola insolens	SEQ ID NO: 2	HIGAL, or HI
Aspergillus aculeatus	SEQ ID NO: 3	AAGAL, or AA
Bacillus licheniformis	SEQ ID NO: 4	BLGAL, or BL

Preferred subgroups of the above are a) MTGAL, HIGAL, AAGAL; b) MTGAL, HIGAL, BLGAL; and c) MTGAL, HIGAL.

In a third embodiment, the parent galactanase has a percentage identity to SEQ ID NO: 1 of at least 25%, using the program ClustalW and the settings referred to above. In further particular embodiments, the percentage identity is at least 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, or at least 95%.

In a fourth embodiment, the galactanase variant has a percentage identity to SEQ ID NO: 1 of at least 50%, using the program ClustalW and the settings referred to above. In further particular embodiments, the percentage identity is at least 55, 60, 65, 70, 75, 80, 85, 90, 95, 97, or at least 99%.

In a fifth embodiment, the parent galactanase has a percentage identity to SEQ ID NO: 2 of at least 25%, using the program ClustalW and the settings referred to above. In further particular embodiments, the percentage identity is at least 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, or at least 95%.

In a sixth embodiment, the galactanase variant has a percentage identity to SEQ ID NO: 2 of at least 50%, using the program ClustalW and the settings referred to above. In further particular embodiments, the percentage identity is at least 55, 60, 65, 70, 75, 80, 85, 90, 95, 97, or at least 99%.

In a seventh embodiment, the parent galactanase has a percentage identity to SEQ ID NO: 3 of at least 25%, using the program ClustalW and the settings referred to above. In further particular embodiments, the percentage identity is at least 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, or at least 95%.

In an eighth embodiment, the galactanase variant has a percentage identity to SEQ ID NO: 3 of at least 50%, using the program ClustalW and the settings referred to above. In

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further particular embodiments, the percentage identity is at least 55, 60, 65, 70, 75, 80, 85, 90, 95, 97, or at least 99%.

In a ninth embodiment, the parent galactanase has a percentage identity to SEQ ID NO: 4 of at least 25%, using the program ClustalW and the settings referred to above. In further particular embodiments, the percentage identity is at least 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, or at least 95%.

In a tenth embodiment, the galactanase variant has a percentage identity to SEQ ID NO: 4 of at least 50%, using the program ClustalW and the settings referred to above. In further particular embodiments, the percentage identity is at least 55, 60, 65, 70, 75, 80, 85, 90, 95, 97, or at least 99%.

In further particular embodiments of each of the above first to tenth embodiments, the alignment is a full Smith-Waterman alignment with the settings referred to above, preferably made with the FASTA package also referred to above.

It is to be understood that also variants of galactanases are contemplated as the parent enzyme.

Preparation of galactanase variants

The galactanase variants may be prepared by any method known in the art, see e.g. Example 1 herein. Typically, a galactanase variant library is prepared. The term "randomized library", "variant library", or simply "library" refers to such library of galactanase variants. Diversity in the variant library can be generated via mutagenesis of the genes encoding the variants at the DNA triplet level, such that individual codons are variegated e.g. by using primers of partially randomized sequence in a PCR reaction. Several techniques have been described, by which one can create a diverse combinatorial library by variegating several nucleotide positions in a gene and recombining them, for instance where these positions are too far apart to be covered by a single (spiked or doped) oligonucleotide primer. These techniques include the use of in vivo recombination of the individually diversified gene segments as described in WO 97/07205 on page 3, lines 8 to 29 (Novozymes A/S). They also include the use of DNA shuffling techniques to create a library of full length genes, wherein several gene segments are combined, and wherein each segment may be diversified e.g. by spiked mutagenesis (Stemmer, Nature 370, pp. 389-391, 1994 and US 5,811,238; US 5,605,793; and US 5,830,721). One can use a gene encoding a galactanase "backbone" (wildtype parent galactanase) as a template polynucleotide, and combine this with one or more single or double-stranded oligonucleotides as described in WO 98/41623 and in WO 98/41622 (Novozymes A/S). The single-stranded oligonucleotides could be partially randomized during synthesis. The double-stranded oligonucleotides could be PCR products incorporating diversity in a specific region. In both cases, one can dilute the

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diversity with corresponding segments encoding the sequence of the backbone galactanase in order to limit the average number of changes that are introduced.

Methods have also been established for designing the ratios of nucleotide mixtures (A; C; T; G) to be inserted in specific codon positions during oligo- or polynucleotide synthesis, so as to introduce a bias in order to approximate a desired frequency distribution towards a set of one or more desired amino acids that will be encoded by the particular codons. It may be of interest to produce a variant library that comprises permutations of a number of known amino acid modifications in different locations in the primary sequence of the polypeptide. These could be introduced post-translationally or by chemical modification sites, or they could be introduced through mutations in the encoding genes. The modifications by themselves may previously have been proven beneficial for one reason or another (e.g. decreasing antigenicity, or improving specific activity, performance, stability, or other characteristics). In such instances, it may be desirable first to create a library of diverse combinations of known sequences. For example, if twelve individual mutations are known, one could combine (at least) twelve segments of the parent protein encoding gene, wherein each segment is present in two forms: one with, and one without the desired mutation. By varying the relative amounts of those segments, one could design a library (of size 212) for which the average number of mutations per gene can be predicted. This can be a useful way of combining mutations, that by themselves give some, but not sufficient effect, without resorting to very large libraries, as is often the case when using 'spiked mutagenesis'. Another way to combine these 'known mutations' could be by using family shuffling of oligomeric DNA encoding the known mutations with fragments of the full length wild type sequence.

The mutated DNA can be expressed by any method known in the art, see e.g. Example 1. Generally, the host cell may be a unicellular microorganism, e.g., a prokaryote, or a non-unicellular microorganism, e.g., a eukaryote.

Useful unicellular cells are bacteria such as Bacillus, Streptomyces, E. coli, Pseudomonas sp., Lactococcus, Lactobacillus, Leuconostoc, Streptococcus, Pediococcus, and Enterococcus,

Examples of eukaryote cells are non-human animal cells, insect cells, plant cells, or fungal cells. Examples of fungal cells are Candida, Hansenula, Kluyveromyces, Pichia, Saccharomyces, Schizosaccharomyces, Yarrowia, Acremonium, Aspergillus, Fusarium, Humicola, Mucor, Myceliophthora, Neurospora, Penicillium, Thielavia, Tolypocladium, and Trichoderma.

Applications

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The galactanase variants of the invention are useful in animal feed, see e.g. WO 97/16982. Non-limiting examples of desirable characteristics of galactanase variants for feed applications are: High temperature stability, acid-stability and high specific activity.

The galactanase variants of the invention may also be used to prepare galacto-oligo-saccharides and for hydrolysis of lactose, both of which are relevant for the dairy industry. For example, the method of Example 5 can be used for screening of galactanase variants for improved activity on lactose, in particular for improved transglycosylation and/or hydrolytic activity on lactose.

The transglycosylation reactions observed with ONPG (Example 4) can be used for screening of galactanase variants for suitable acceptor affinities. The screening may be a high-through-put screening. This provides valuable knowledge of the affinities of the individual subsites (such as subsites +1, +2, +3, +4) for various acceptors, e.g. galactose (Gal), ß-1,4-galactobiose (Gal2) (Megazyme), ß-1,4-galactotriose (Gal3), ß-1,4-galactotetraose (Gal4), glucose (Glu), arabinose (Ara), galacturonic acid (GalA), maltose (Mal) or maltotriose (Mal3).

The results of Example 3 provides knowledge of individual subsites for galactose (-3 to +3), as well as knowledge of the tendencies to transglycosylate instead of hydrolyse substrates. This knowledge is useful for the designing of galactanase variants of desired properties.

Various references are cited herein, the disclosures of which are incorporated by reference in their entireties.

EXAMPLES

Example 1: Preparation of galactanase variants

The D181N mutation was introduced in the AAGAL encoding gene by the use of the mutagenic oligonucleotide 5'- CAT TTG GAC AAC GGC TGG AGC -3' (SEQ ID NO: 5) and the mega-priming method described by Sarkar, G., and Sommer, S.S., 1990. The "Megaprimer" Method of Site-Directed Mutagenesis. BioTechniques, 8: 404-407. The mutations D181N+S90A+D91H were introduced in a similar way.

The resulting variant genes were cloned into plasmid pHD464 as desribed in Dalbøge H., Heldt-Hansen H. 1994. A novel method for efficient expression cloning of fungal enzyme genes. Mol. Gen. Genet. 243: 253-260, and the correct introduction of the mutations were verified by DNA sequencing.

The A90S+H91D double mutation was introduced in the MTGAL encoding gene essentially as described above by the use of the mutageneic oligonucleotode 5'- GCC GAT CCT TCT GAT CAG ACC ATG CC -3' (SEQ ID NO: 6).

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Proteins were expressed in, and secreted from Aspergillus oryzae essentially as described in Christensen, T., Wöldike, H., Boel, E., Mortensen, S.B., Hjortshøj, K., Thim, L., Hansen, M.T., 1988. High level expression of recombinant genes in Aspergillus oryzae. Bio/Technology 6, 1419-1422.

5 Example 2: Purification and characterization of galactanase variants

Purification of Aspergillus aculeatus galactanase variants

The culture supernatant from a fermentation of the Aspergillus oryzae strain expressing the site-directed recombinant Aspergillus aculeatus galactanase variant D181N (described in Example 1) was filtered through a 0.22 µm filter to remove the mycelia. 1200 ml filtrate was added ammonium sulphate to a concentration of 1.6 M, loaded onto a 50 ml butyl column equilibrated with 25 mM sodium acetate, 1.6 M ammonium sulphate pH 5.0 and eluted using a linear ammonium sulphate decreasing from 1.6 M to 0 M over 10 column volumes. Galactanase activity was measured by mixing 40 µl of fractions with 200 µl 10 mg/ml lupin AZCL-galactan (Megazyme, Australia) in 0.5 M MES pH 6.5 After about 30 min incubation at room temperature, insoluble substrate was removed by centrifugation, and absorbance of supernatant measured at 590 nm. Fractions containing galactanase activity eluted around 1 M ammonium sulphate were pooled and dialysed against 10 mM sodium citrate pH 3.5. Dialysate (400 ml) was diluted to 2000 ml with water and loaded onto a 50 ml S-Sepharose column equilibrated with 10 mM sodium citrate pH 3.5. Galactanase activity did not bind to this column and was concentrated to 80 ml on an Amicon ultrafiltration device. with a 10 kDa cut off filter. The concentrate was at least 95% pure estimated from SDS-PAGE.

The culture supernatant from a fermentation of the Aspergillus oryzae strain expressing site-directed recombinant Aspergillus aculeatus galactanase variant D181N+S90A+D91H was filtered as described above. 900 ml filtrate was added ammonium sulphate to a concentration of 1.6 M, and eluted from a 50 ml butyl column as described above. Galactanase activity was measured as described above. Fractions containing galactanase activity eluted around 0.35 M ammonium sulphate and were pooled and dialysed against 25 mM sodium acetate pH 5.5. Dialysate (200 ml) was diluted to 275 ml with water, loaded onto a 50 ml Q-Sepharose column equilibrated with 25 mM sodium acetate pH 5.5, and eluted with a linear gradient from 0 to 1 M NaCl over 10 column volumes. Fractions containing galactanase activity (around 0.8 M NaCI) were pooled and concentrated to 10 ml on an Amicon ultrafiltration device with a 10 kDa cut off filter. The concentrate was at least 95% pure estimated from SDS-PAGE.

Purification of Myceliophthora thermophila galactanase variants

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The culture supernatant from a fermentation of the Aspergillus oryzae strain expressing the site-directed recombinant Myceliophthora thermophila galactanase variant A90S+H91D (described in Example 1) was filtered through a 0.22 µm filter to remove the mycelia. 1200 ml filtrate was added ammonium sulphate to a concentration of 1.6 M, loaded onto a 50 ml butyl column equilibrated with 25 mM sodium acetate, 1.6 M ammonium sulphate pH 5.0 and eluted using a linear ammonium sulphate decreasing from 1.6 M to 0 M over 10 column volumes. Galactanase activity was measured by mixing 40 µl of fractions with 200 µl 10 mg/ml lupin AZCL-galactan (Megazyme, Australia) in 0.5 M MES pH 6.5 After about 30 min incubation at room temperature, insoluble substrate was removed by centrifugation, and absorbance of supernatant measured at 590 nm. Fractions containing galactanase activity eluted around 1 M ammonium sulphate were pooled and dialysed against 10 mM sodium citrate pH 3.5. Dialysate (400 ml) was diluted to 2000 ml with water and loaded onto a 50 ml S-Sepharose column equilibrated with 10 mM sodium citrate pH 3.5. Galactanase activity did not bind to this column and was concentrated to 80 ml on an Amicon ultrafiltration device with a 10 kDa cut off filter. The concentrate was at least 95% pure estimated from SDS-PAGE.

Characterization of the purified variants

The pH profiles of the purified variants described above were established as follows: Galactanase activity at various pH was measured by mixing 500 µl 4 mg/ml lupin AZCL-galactan (Megazyme, Australia) in water with 500 µl buffer (50 mM sodium acetate, 50 mM potassium dihydrogenphosphate, 50 mM boric acid, 1 mM CaCl₂, 0.01% Triton X-100 adjusted to pH 2.5, 3.5, 4.5, 5.5, 6.5, 7.5, 8.5 or 9.5 with HCl/NaOH) and 25 µl purified enzyme diluted to about 0.5-2 µg/ml in water. The mixture was incubated 15 min at 37°C, insoluble material was removed by centrifugation, and absorbance in the supernatant was measured at 590 nm.

From the results shown in Table 1 below, it appears that the pH profiles have changed (the profile of the AAGAL variants D181N, and D181N+S90A+D91H have been shifted to the alkaline side; and the pH profile of the MTGAL variant A90S+H91D has been shifted to the acidic side, as compared to the wild types).

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Table 1								
Galactanase / pH	2.5	3.5	4.5	5.5	6.5	7.5	8.5	9.5
AAGAL	73	100	83	47	32	0	2	0
AAGAL D181N	74	99	100	87	74	35	7	0
AAGAL D181N+S90A+D91H	55	59	71	83	100	90	21	0
MTGAL	0	12	41	63	90	100	54	7
MTGAL A90S+H91D	0	8	51	75	100	95	35	4

Example 3: Activity on galactooligosaccharides

Preparation of galactotriose (Gal3), galactotetraose (Gal4), methyl-galactotrioside (MeGal3) and methyl-galactotetraoside (MeGal4)

Galactan (lupin) was purchased from Megazyme. All solvents, reagents and TLC-plates (Silica gel 60 F_{254}) were purchased from Merck. ¹H NMR spectra were recorded on a Varian Mercury 400 MHz at 30°C. As reference values CHCl₃ in CDCl₃ (7.27 ppm) and HDO in D₂O (4.67 ppm) were used. Flash chromatography was accomplished using a FLASH 40i chromatography module from Biotage.

<u>Undeca-O-acetyl galactotriose</u>: Arabinofuranosidase treated lupin galactan (0.50 g) was dissolved in 10 mM Bis-Tris buffer pH 6.5 (50 mL) by stirring for 1 h at 37°C. BLGAL was added (250 GalU/mL) and the solution stirred for 3 h at 37°C and then 5 min at 100°C. TLC (eluent: propanol/ethanol/H₂O (7:1:2)) showed a major (Gal3) and a minor product (Gal4) both eluting below commercial galactobiose. After cooling, the solution was concentrated, dried and acetylated and worked up by standard procedures ($Ac_2O/pyridine$, 48 h at room temperature (rt)). The crude product was purified by flash chromatography (eluent: EtOAc/heptane 5:2) to give 0.20 g of pure Gal3 peracetate (mixture of alpha- and beta-anomer (1:2)). ¹H NMR (selected data, CDCl₃): 6.29 ppm (d, $J_{1,2}$ = 3.5 Hz, H-1alpha), 5.63 ppm (d, $J_{1,2}$ = 8.4 Hz, H-1ß).

Galactotriose (Gal3): Deacetylation of the acetylated triose was accomplished by stirring overnight in methanol/NaOCH₃ (1 mL 1M NaOCH₃ in 3 mL methanol) and then neutralized by addition of Dowex 50 Wx8. Water (2 mL) was added and the resin removed by filtration. The clear solution was concentrated (freeze-drying) to give 0.10 g of solid G3. MS (MALDI-TOF): 527 (M+23, Na). ¹H NMR (selected data, D₂O): 5.20 ppm (d, J = 3.6 Hz, H-1alpha), 4.5-4.6 (3 x d, H-1G, H-1', H-1").

Methyl deca-O-acetyl galactotrioside: The acetylated galactotriose (0.24 g) was converted into the bromide by treatment (5 h) with 30% HBr in acetic acid (2.5 mL) and CH_2Cl_2 (2 mL) at 0°C \rightarrow rt. The reaction was worked up by standard procedures and concentrated to give a yellowish syrup (194 mg) of the alpha-bromo compound, which was used without further purification. 1H NMR (selected data, CDCl₃): 6.57 ppm (d, 1H, $J_{1,2} = 3.8$ Hz, H-1). The bromo-glycoside (0.19 g, 0.20 mmol) was converted into the methyl glycoside by overnight

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treatment with Ag_2CO_3 (60 mg, 22 mmol) in dry methanol (10 mL) (under nitrogen). After work up, the methyl glycoside was purified by flash chromatography (eluent: EtOAc/heptane (3:1)) to give 30 mg of pure compound (colorless oil). ¹H NMR (selected data, CDCl₃): 4.48 ppm, 4.39 ppm and 4.35 ppm (3xd, 3H, $J_{1,2}$ = 8.0 Hz, H-1, H-1' and H-1"), 3.47 ppm (3H, s, OCH₃).

Methyl galactotrioside (MeGal3): The acetylated methyl glycoside (30 mg) was deacetylated as described above to give 10 mg of syrupy material.

<u>Galactotetraose (Gal4)</u>: This was prepared as described for Gal3 using 100 GalU/mL. Yield of final deacetylated product: 17 mg..

Methyl galactotetraoside (MeGal4): This compound was prepared in analogy with MeGal3 and 41 mg of MeGal4 was obtained from 1 g of galactan. MS (MALDI-TOF): 704 (M+23, Na).

Activity of HIGAL, MTGAL, AAGAL and BLGAL on galactooligosaccharides

The activity on the galacto-oligosaccharide substrates prepared as described above and on the commercially available galactobiose (Gal2, Megazyme) was studied for the four purified galactanases HIGAL, MTGAL, AAGAL and BLGAL. The buffers and temperatures used were: 25 mM sodium acetate, 0.5 mM CaCl₂, 0.005 % Triton X-100, pH 6.5 at 37°C for HIGAL and MTGAL, 50 mM sodium acetate, 1 mM CaCl₂, pH 4 at 30°C for AAGAL and 50 mM Mes, 1 mM CaCl₂, pH 6.5 at 30°C for BLGAL. Enzyme concentrations used were 0.8 µg/ml for HIGAL, 0.2 µg/ml for MTGAL, and 10 µg/ml for AAGAL and BLGAL. With HIGAL and MTGAL substrate concentrations were all 0.25 mg/ml, whereas 0.34 mg/ml Gal2, 0.050 mg/ml Gal3 and 0.067 mg/ml Gal4 were used for AAGAL and BLGAL. Enzyme activity in samples withdrawn after various incubation times was inactivated by heating to 95°C for 10 min. Compositions of reaction products were analysed using HPAE-PAD (Dionex) applying a PA-100 column and a linear gradient of sodium acetate (0-0.18 M) in 0.15 M NaOH. Response factors of the individual carbohydrates were estimated from reference runs with MeGal3, MeGal4, Gal, Gal2, Gal3 and Gal4. Selected results are shown in Tables 2-8 below (the figures indicating weight percentage of glactooligosaccharides).

Neither of the enzymes HIGAL, MTGAL, AAGAL or BLGAL had any detectable activity on Gal2 in 24 hours. HIGAL, MTGAL and AAGAL degraded Gal3 to Gal2 and Gal, whereas BLGAL had no visible activity on Gal3 after 24 hours. Incubation of HIGAL and MTGAL with MeGal3 (See Tables 2 and 3) gave much higher release of MeGal than MeGal2, indicating that Gal is released from the reducing end of Gal3 with both enzymes.

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HIGAL and MTGAL degraded Gal4 (also containing about 40% Gal3) (Tables 4 and 5) mainly to Gal and Gal2, whereas Gal3 did not accumulate. Results for HIGAL and MTGAL with MeGal4 (Tables 6 and 7) gave initial release mainly of MeGal, MeGal2 and Gal3 and some Gal2 but little Gal, again indicating that Gal is released mainly from the reducing end of Gal4. The production of Gal from MeGal4 in the later stages of the hydrolysis may be mainly due to hydrolysis of transglycosylation products with no methyl group at the reducing end. BLGAL degrades galactotetraose mainly to galactose and galactotriose. With MeGal4 the main products from BLGAL were MeGal and Gal3, indicating that Gal is released from reducing end of Gal4. With AAGAL the initial products from galactotetraose are about equimolar amounts of galactose, galactobiose and galactotriose, but subsequently the galactotriose is degraded to galactobiose and galactose.

Table 2: Degradation of MeGal3 with HIGAL

Incubation				1	
time (hours)	0.0	0.5	2.2	5.0	72.0
Gal	0.0	0.0	2.3	3.0	17.1
Gal2	0.0	3.9	12.5	20.2	36.2
Gal3	0.0	1.2	3.3	10.6	8.0
MeGal	0.0	11.4	18.4	36.8	34.6
MeGal2	0.0	3.3	3.7	5.2	4.2
MeGal3	100.0	80.3	59.7	24.2	0.0

15 Table 3: Degradation of MeGal3 with MTGAL

Incubation		,			
time (hours)	0.0	0.5	2.2	5.0	72.0
Gal	0.0	. 0.0	14.1	2.2	6.5
Gal2	0.0	0.0	8.5	10.9	37.2
Gal3	0.0	0.0	0.4	15.7	23.2
MeGal	0.0	10.1	27.6	17.4	28.3
MeGal2	0.0	2.7	1.9	3.2	3.5
MeGal3	100.0	87.2	47.5	50.6	1.3

Table 4: Degradation of Gal4 with HIGAL

Incubation	1		}	1	}
time (hours)	0.0	0.5	2.2	5.0	72.0
Gal	0.0	5.8	16.7	35.6	65.2
Gal2	0.0	8.1	21.9	34.8	33.6

Gal3	42.0	43.2	39.8	23.9	0.9
Gal4	58.0	42.9	21.6	5.7	0.2

Table 5: Degradation of Gal4 with MTGAL

Incubation	}	}		İ	
time (hours)	0.0	0.5	2.2	5.0	72.0
Gal	0.0	11.6	14.9	29.2	54.9
Gal2	0.0	9.9	17.4	29.1	43.5
Gal3	42.0	27.7	45.5	29.5	1.5
Gal4	58.0	50.8	22.3	12.1	0.0

Table 6: Degradation of MeGal4 with HIGAL

incubation	1		1		}
time (hours)	0.0	0.5	2.0	5.0	24.0
Gal	0.0	2.3	1.6	7.4	26.4
Gal2	0.0	6.3	5.0	13.8	25.3
Gal3	0.0	20.6	16.0	19.7	9.1
Gal4	0.0	3.3	3.2	3.2	1.7
MeGal	1.6	12.1	10.5	16.6	19.1
MeGal2	4.7	12.6	13.2	16.1	13.4
MeGal3	14.8	17.2	18.4	15.5	5.0
MeGal4	79.0	25.5	32.1	7.6	0.0

Table 7: Degradation of MeGal4 with MTGAL

Incubation	1	1	1	1	1
time (hours)	0.0	0.5	2.0	5.0	24.0
Gal	0.0	0.9	4.8	12.4	24.2
Gal2	0.0	3.3	10.9	20.1	32.7
Gal3	0.0	13.7	23.9	17.9	3.4
Gal4	0.0	2.5	3.7	2.9	1.1
MeGal	1.6	8.9	16.2	19.3	20.1
MeGal2	4.7	9.6	. 13.6	13.9	13.3
MeGal3	14.8	17.1	16.0	9.9	2.3
MeGal4	79.0	43.9	10.9	3.5	2.9

Example 4: Activity with o-nitrophenyl-ß-D-galactopyranoside (ONPG)

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The activity of HIGAL and MTGAL with ONPG was tested by mixing 200 µl (normally 5.5 mg/ml) ONPG in 50mM sodium acetate, 1 mM CaCl₂, 0.01% Triton X-100, pH 6.5 with 25 µl galactanase (normally 1 mg/ml) in the well of a microtiter plate. Release of o-nitrophenol (ONP) was measured at room temperature at 405 nm every 10 seconds normally for 30 min on a SpectraMaxPlus (Molecular Devices). Effects on the observed release of ONP was studied with varied enzyme concentration, ONPG concentration and with addition of galactose (Gal), β-1,4-galactobiose (Gal2) (Megazyme), β-1,4-galactotriose (Gal3), β-1,4-galactotriose (Gal4), glucose (Glu), arabinose (Ara), galacturonic acid (GalA), maltose (Mal) or maltotriose (Mal3).

In Tables 8-11 below, incubation times required to increase the observed absorbance at 405 nm by given amounts are listed. Cells marked 'n.r.' indicate that the increase in absorbance was not reached in the experiment. In general, the initial increase in absorbance at 405 nm was very slow, but after a lag phase the rate of ONP release often increased drastically - often approximately exponentially. The most likely explanation for the observed kinetics is that ONPG reacts with the enzyme to give an enzyme-galactosyl intermediate which hydrolyses very slowly. Instead, the Gal of the intermediate is released by transglycosylation, initially with ONPG or added sugar as acceptor. In cases where the rate of ONP release increases, these transglycosylation products are even better acceptors than the intiglespeer in Table 8, the rate of ONP release is about proportional to the amount of added enzyme. HIGAL releases ONP faster than MTGAL at identical enzyme dosage. Addition of Gai (5 mg/ml) is seen to slow the ONP release by about a factor of two for MTGAL and a factor of three for HIGAL. Probably, Gal does not significantly slow formation of the enzyme-galactosyl intermediate, which would accumulate even if Gal had high affinity for the -1 or +1 subsite. More likely, Gat inhibits the subsequent transglycosylation, which requires binding of ONPG to the +1 and +2 subsites, e.g. by binding to the +2 subsite. With 50 mg/ml Gal added (results not shown) release of ONP was even slower with only insignificant increase of absorbance at 405 nm in 30 min.

The results in Table 9 show that rate of ONP release is similar with 5 and 10 mg/ml ONPG but slower at 2.5 and especially 1.25 mg/ml ONPG. This indicates that the rate-limiting transglycosylation reaction with ONPG as acceptor has a Km of about 3 mg/ml.

In Table 10 effects of adding 0.5 or 0.05 mg/ml Gal2, Gal3 or Gal4 are given. Contrary to Gal each of these three galactooligosaccharides increases the rate of ONP release. The initial ONP release rates indicate that Gal4 is more efficient than Gal3 as acceptor, and that Gal3 is more efficient than Gal2. With Gal2 and Gal3, ONP release rate increases significantly with incubation time, indicating that transglycosylation products (initially Gal3 and Gal4, respectively) are more efficient acceptors than the added sugars, whereas the release rate is relatively constant with Gal4. These results indicate that HIGAL possesses four significant subsites (+1,+2, +3,+4) on the reducing side of the cleaved bond.

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In Table 11 results upon addition of Glu, Ara, Mal, Mal3 and GalA are given. As experiments were run on three different days, and ONP release rate even in Identical experiments had been seen to vary slightly (possibly due to variants in temperature), results with only ONPG and HIGAL added run in the same three experiments are shown. It is seen that 5 mg/ml Ara inhibits the transglycosylation, resulting in about three times slower ONP release. 5 mg/ml Glu also has slight inhibitory effect, whereas 50 mg/ml Glu (results not shown) resulted in very little ONP release (<0.02) in 30 min. As with Gal, this indicates binding of these sugars to subsites in the enzyme-galactosyl intermediate, which prevents ONPG to act as acceptor and where the sugars themselves also has little or no acceptor fucntion. With 5 mg/ml Mal or Mal3 no significant effects on ONP release are observed. 5 mg/ml GalA has weak inhibitory effect, whereas 50 mg/ml GalA slows ONP release by about a factor two. From these results ranking of the inhibitory effect of the tested sugars is: Gal ~ Ara > Glu > GalA > Mal = Mal3 = 0.

Using HPAE-PAD chromatography (Dionex LC-500 System, PA-100 column, linear gradient of 0-0.6 M sodium acetate in 100 mM NaOH), the production of larger oligosaccharides from transglycosylation upon incubation of HIGAL (110 µg/ml) at room temperature (0.5 to 14 min followed by heat inactivation for 10 min at 95°C resulting in A₄₀₅: 0.15-0.67) in 50 mM sodium acetate, 1 mM CaCl₂, 0.01% Triton X-100, pH 6.5 with ONPG (5 mg/ml) with and without Gal2 (0.05 mg/ml) or Gal3 (0.05 mg/ml) as acceptor was verified.

Table 8: Rate of ONP release, MTGAL and HIGAL in varying dosages, and +/- sugar

MTGAL:	MTGAL:	MTGAL:	MTGAL:	MTGAL:	HIGAL:	HIGAL:	HIGAL:	HIGAL:	HIGAL:
110	55	28	110	55	110	55	28	110	55
-			Gal: 5	Gal: 5				Gal: 5	Gal: 5
14.0			26.9	40.2	9.0	20.4	41.4	32.0	57.0
20.5			44.5	n.r.	10.3	22.9	46.5	35.7	n.r.
26.4			n.r.	n.r.	11.5	25.4	51.0	41.5	n.r.
31.4		n.r.	n.r.	n.r.	12.7	28.0	56.5	46.7	n.r.
34.5			n.r.	n.r.	13.8	30.9	n.r.	52.7	n.r.
39.2			n.r.	n.r.	15.0	32.0	n.r.	59.0	n.r.
43.9 r				n.r.	15.0	35.0	n.r.	n.f.	n.r.
46.7					17.7	37.9	n.r.	n.r.	n.r.
0 10 14 14 10 10 10 10		29.9 29.9 0.1. 0.1. 0.1.	9 40.4 5 n.r. n.r. n.r. n.r.	Gal: 5 9 40.4 26.9 5 n.r. 44.5 7 n.r. n.r. n.r. n.r. n.r. n.r. n.r. n.r	Gal: 5 9 40.4 26.9 5 n.r. 44.5 7 n.r. n.r. n.r. n.r. n.r. n.r. n.r. n.r	Gal: 5 Gal: 5 9 40.4 26.9 40.2 5 n.r. 44.5 n.r. 5 n.r. n.r. n.r. n.r. n.r. n.r. n.r. n.r.	Gal: 5 Gal: 5 Gal: 5 9 40.4 26.9 40.2 9.0 20.4 5 n.r. 44.5 n.r. 10.3 22.9 5 n.r. n.r. 11.5 25.4 5 n.r. n.r. 17.7 28.0 n.r. n.r. 13.8 30.9 n.r. n.r. 15.0 32.0 n.r. n.r. 15.0 35.0 n.r. n.r. 17.7 37.9	Gal: 5 Gal: 5 Gal: 5 9 40.4 26.9 40.2 9.0 20.4 5 n.r. 44.5 n.r. 10.3 22.9 5 n.r. n.r. 11.5 25.4 5 n.r. n.r. 12.7 28.0 n.r. n.r. n.r. 13.8 30.9 n.r. n.r. 15.0 32.0 n.r. n.r. 15.0 35.0 n.r. n.r. 17.7 37.9	9 40.4 26.9 40.2 9.0 20.4 41.4 32.0 5 n.r. 44.5 n.r. 10.3 22.9 46.5 35.7 5 n.r. n.r. 11.5 25.4 51.0 41.5 6 n.r. n.r. 12.7 28.0 56.5 46.7 7 n.r. n.r. 13.8 30.9 n.r. 52.7 8 n.r. n.r. 15.0 32.0 n.r. 59.0 9 n.r. n.r. 15.0 35.0 n.r. n.r. 0.r. n.r. n.r. 17.7 37.9 n.r. n.r.

Table 9: Rate of ONP release at varying ONPG concentrations

Table 3. Ivale of O'NT Telease at Varying O'NT'G Concentrations	II VIII OINPO CONCENITATI	Suo	_	•	
Enzyme: µg/mi		HIGAL: 110	HIGAL: 110	HIGAL: 110	HIGAL: 110
ONPG (mg/ml)		10	5	2.5	1.25
Sugar: mg/ml					
Time (min) to increase A405 by: 0.025		6.3	6.0	9.7	28.7
	0.05	7.7	8.0	11.3	n.r.
	0.1	8.8	9.2	12.7	n.f.
	0.2	10.0	10.2	14.0	n.f.
	0.4	11.2	11.3	15.5	חינ.
	0.8	12.3	12.5	17.3	n.r.
	1.6	13.5	13.8	19.5	n.r.
	3.2	14.7	15.3	22.8	n.r.
	-	-	-		

Table 10: Rate of ONP release, addition of various amounts of various galactooligosaccharides

) UICAL.	1110 41 .				(
		TIGAL:	HIGAL:		HIGAL:		HIGAL:	HIGAL:
Enzyme: µg/ml		110	110	HIGAL: 110	110	HIGAL: 110	110	110
ONPG (mg/ml)		5	5	5	5	5	5	5
Sugar: mg/ml			Gal2: 0.5	Gal2: 0.05	Gal3: 0.5	Gal3: 0.05	Gal4: 0.5	Gal4: 0.05
Initial rate (mOD/min)		6.0	9	2	200	40	. 002	80
Time (min) to increase A405 by:	0.025	10.0	2.7	5.5	0.0	0.5	0.0	0.2
	0.05	11.3	3.5	6.8	0.2	1.0	0.0	0.5
	0.1	12.8	4.8	8.2	0.3	1.7	0.0	0.8
	0.2	14.2	6.0	9.5	0.5	2.3	0.2	1.5
	0.4	15.7	7.2	10.7	0.8	3.3	0.5	2.5
	9.0	17.0	8.3	11.8	1.5	4.8	1.0	3.7
	1.6	18.5	9.7	13.3	2.5	6.3	2.2	5.2
	3.2	20.0	11.0	15.2	3.8	7.7	5.3	7.5

Table 11: Rate of ONP release, inhibition by sugars

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		HIGAL:	HIGAL:	HIGAL:	HIGAL:	HIGAL:	HIGAL:	HIGAL:	HIGAL:	HIGAL:
Enzyme: µg/ml		110		110	110	110	110	110	110	110
ONPG (mg/ml)		5	5	5	5	S	5	5	5	5
Sugar: mg/ml			Glu: 5	Ara: 5		Mal: 5	Mal3: 5		GalA: 50	GalA: 5
Time (min) to increase A405 by: 0.025	0.025	8.5	12.8	26.5	11.0	11.5	11.0	8.7	13.7	9.5
	0.05	9.5	14.8	n.r.	12.5	13.0	12.3	9.8	16.7	11.2
	0.1	10.8	17.0	n.r.	13.8	14.3	13.8	11.0	20.0	12.7
	0.2	12.0	19.3	n.r.	15.2	15.7	15.2	12.2	23.3	14.3
	0.4	13.3	21.8	n.r.	16.5	17.2	16.5	13.3	26.8	15.8
J. Time.	9.0	14.5	24.3	n.r.	18.0	18.7	18.0	14.7	n.r.	17.5
	1.6	15.8	27.0	n.f.	19.5	20.2	19.3	16.0	n.f.	19.3
	3.2	17.3	n.r.	n.r.	21.3	22.0	21.3	17.3	n.r.	22.5

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Example 5: Activity on lactose

HIGAL (60 μg/ml) and MTGAL (750 μg/ml) were incubated at 50°C with lactose (Lac) (100 mg/ml) at pH 4.8 (25 mM sodium citrate), 6.45 (25 mM sodium acetate, 0.5 mM CaCl₂, 0.005% Triton X-100) and 8.6 (50 mM Tris, 0.01 % Brij 35). 20 μl samples were withdrawn after 2, 23 and 120 hours, 980 water added and enzyme inactivated by heating to 95°C for 10 min. After a further 20 time dilution with water, samples were analysed using HPAE-PAD (Dionex LC-500 system, PA-100 column, 0-3 min: 150 mM NaOH, 3-19 min: linear gradient 0-0.18 M sodium acetate in 150 mM NaOH). Response factors for the individual peaks were estimated from standards of Gal, Glu, Lac, Gal2, Gal3 and Gal4.

Under these conditions only MTGAL at pH 4.5 and 6.5 gave significant conversion of Lac. In Tables 12 and 13 weight fractions of the analysed products with MTGAL at pH 4.5 and 6.45 are given. The figures indicate weight% of the products resulting from the incubation. The term DP3 indicates transglycosylation product consisting of three sugar units, and the term DP4+ transglycosylation products consisting of four or more sugar units. Unfortunately, the analysis method used was not able to separate Glu and Gal.

With transglycosylation occurring according to the reaction:

the weight fraction of DP3 should be about three times higher than the weight of the monomer. After 2 hours the ratio is about 1.5 at both pH's indicating that this is not the only reaction taking place. The production of larger oligosaccharides (DP4+) is a result of the initial transglycosylation product functioning as acceptor for further transglycosylation:

Also, from the increasing amount of Gal/Glu without corresponding increase in transglycosylation products (DP3 and DP4+) after 23 and 120 hours, it is evident that hydrolysis of transglycosylation products takes place. These hydrolysis reactions seem to be slower at pH 6.45 than at pH 4.5.

Table 12: Activity of MTGAL on lactose (pH 4.5)

Incubation ti (hours)	ime 2	23	120	
Glu/Gal	1.4	12.5	38.8	
Lac/Gal2	96.0	78.7	51.2	
DP3	2.0	7.0	8.9	
DP4+	0.5	1.8	1.1	

Table 13: Activity of MTGAL on lactose (pH 6.45)

Incubation time (hours)	2	23	120
Glu/Gal	1.0	6.5	21.0
Lac/Gal2	95.7	85.3	62.6
DP3	1.4	6.3	11.7
DP4+	1.9	1.9	4.7

Example 6: Activity on galactan

Lupin galactan (Megazyme) was incubated with BLGAL (0.1-10 μg/ml) at pH 6.5 (50 mM MES, 1mM CaCl2) and with AAGAL (0.1-10 μg/ml) at pH 4.0 (50 mM sodium acetate, 1 mM CaCl2) at 30°C. Samples were withdrawn after 45 min to 24 hours and enzyme inactivated by heating to 95°C for 10 min. Reaction products were analysed using HPAEC-PAD on a Dionex chromatographic system using a CarboPac PA-100 column and a linear gradient 0 to 0.3 M sodium acetate in 0.15 M NaOH. Purified galacto-oligosaccharides were used to identify products.

With BLGAL the initial main product is galactotetraose with both smaller and larger oligomers also present. Upon longer incubation the fractions of galactose, galactobiose and galactotriose increase and after prolonged incubation only these three oligomers are seen in molar ratios of about 1:0.4:0.9.

AAGAL initially produces a more homogeneous mixture of galactooligomers. Further degradation yields mainly galactose, galactobiose and galactotriose, and finally almost exclusively galactose and galactobiose are seen in a molar ratio of about 2:1. Small peaks probably corresponding to galactobioses and galactotrioses resulting from transglycosylation reactions with glucosidic bonds different from ß-1,4 are also present.

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CLAIMS

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and

1. A variant of a parent Glycoside Hydrolase Family 53 galactanase, comprising an alteration in at least one of the following positions: -6, -4, -2, 1, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 18, 20, 22, 24, 25, 26, 29, 30, 31, 32, 36, 39, 40, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 54a, 54e, 54f, 54g, 54h, 55, 56, 57, 58, 61, 62, 65, 69, 77, 79, 80, 81, 82, 5 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 101, 106, 107, 110, 113, 114, 126, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 144, 145, 146, 147, 150, 153, 157, 159, 163, 169, 171, 172, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 191, 192, 194, 198, 200, 203, 204, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234, 241, 10 242, 243, 244, 245, 246, 247, 248, 249, 250, 252, 252d, 252e, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 265, 266, 273, 274, 276, 277, 280, 283, 284, 286, 288, 288a, 289, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301, 302, 302a, 302d, 302j, 302k, 302m, 302n, 302o, 302q, 302r, 302s, 302t, 302u, 302v, 302x, 302y, 302z, 302aa, 302bb, 302cc, 302dd, 302ee, 302ff, 302gg, 302hh, 302ii, 302jj, 303, 304, 305, 306, 307, 308, 309, 310, 311, 15 312, 313, 314, 315, 316, 317, 318, 319, 320, 321, 322, 323, 324, 325, 326, 327, 328, 329, and 330; wherein

(a) the alteration(s) are independently

- (i) an insertion of an amino acid immediately downstream of the position,
- (ii) a deletion of the amino acid which occupies the position, and/or
- (iii) a substitution of the amino acid which occupies the position;
- (b) the variant has galactanase activity.
- 36A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 39C; 40C; 41P; 43A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 44A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 46A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 48A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 49A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 50A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 51A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 52A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 53A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

- 54aP; 54eA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 54fA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 54gA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 54hA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 55A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- 56A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 57A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 58A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 61A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 62C; 65C; 69C; 77A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - 79A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 80A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 81A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- 93A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 94A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 95A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 96A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 97P;
 101P;
 106C;
 107H,S;
 113C;
 114C;
 126E;
 - 131A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - 133A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- 25 134A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - 135A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - 136A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 137A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - 139A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- 30 140A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - 141A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - 142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 144P;
 - 146A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 147P; 150C; 159C; 163C; 169P; 171P;
 - 172P; 178A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- 35 179A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - 180A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - 181A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - 182A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

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- 183A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      184A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      185A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      186A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      187A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
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      188A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      189A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      191A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      194C; 198P; 200P; 203P; 204P; 210A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
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     211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     213A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     215A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
15
     216A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 216FVASTG;
     217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     218A.C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     219A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     220A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
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     221A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     222A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     223A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     224A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     225A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
25
     226A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     227A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     228A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     229A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     230A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     231A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
30
     232A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     233A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     234C; 241A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     242A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
    243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     244A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     245A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
    246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
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247A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y:
     249A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     250A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     252A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 5
     252dA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     252eA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     253A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     254A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
10
     255A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     256A,C,D,E,F,G,H,1,K,L,M,N,P,Q,R,S,T,V,W,Y;
     257A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     258A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     259A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
15
     260A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     261A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     262A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     263A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     264A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     265A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
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     266P; 273A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 274C;
     276A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     277A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     280A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     283A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 286P; 288P; 288aP; 289P;
25
     293A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     294A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     297A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
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     298A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     299A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     300A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     301A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
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     302A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     302aA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302dP;
     302jA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
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302kA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302mA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302nA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302oA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302qA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 5 302rA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302sA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302tA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302uA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;302vA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 302xA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y, 302yA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302zA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302aaA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302bbA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302ccP; 15 302ddA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;302eeA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302ffA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302ggA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302hhA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 302iiA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 302jjA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 303A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 304A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 305A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 25 306A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 307A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 308A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 309A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 310A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 311A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 312A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 313A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 314A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 315A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 316A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 317A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 318A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

319A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
320A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
321A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
322A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
323A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 324P; 325P;
326A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 327P; 328C;
329A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; and/or 330C.

- 3. The variant of any one of claims 1-2, wherein the variant comprises at least one of the following substitutions: *-6P; *-4P; *-2P; A1P; T3P; R5A.C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V7A,C,D,E,F,G,H,İ,K,L,M,N,P,Q,R,S,T,W,Y; D8A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S9A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
- V13A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V14A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; E15A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E16A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A18C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V20A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N24C,P; T25P; N26P; A29P; Q30C; L32A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
- 20 L36A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; N39C; G40C; V41P; T43A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; V44A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Q46A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; R47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; V48A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; W49A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; V50A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
- N51A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A53C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D54A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *54aP; *54eA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 54fA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - *54gA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- *54hA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 G55A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 N56A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
 Y57A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 Y61A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
- N62C; I65C; A69C; Y77A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
 D79A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F80A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y82A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
 S83A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; D84A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

T85A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,,V,W,Y; W86A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; A87C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D88A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A90C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H91A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q92A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T93A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; M94A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; 95A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A96C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G97P; D101P; S106C; W107H,S; Y110C; T113C; L114C; Q126E; 131A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G133A,C.D.E.F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 10 E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; I136A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; R137A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y: G139A.C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 L140A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L141A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; W142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; T144P; R146A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; T147P; W150C; S159C; G163C; 169P; K172P; H178A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 179A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D180A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 N181A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; G182A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W183A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; D184A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W185A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; 25 G186A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T187A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y: Q188A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; N189A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W191A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;N194C; Q198P; T200P; L203P; S204P; 30 G210A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; S212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; F213A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; 35 P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F216FVASTG;

Y217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;

S218A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S219A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S220A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; A221C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 5 T222A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S224A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; A225C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L226A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 10 K227A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; S228A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; \$229A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; L230A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D231A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N232A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 15 M233A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; A234C; 1241A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; A242C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V244A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 20 E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; N247A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y: W248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; P249A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 25 1250A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; C252A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *252dA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *252eA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P253A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 30 N254A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; P255A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; R256A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Y257A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S258A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 35 F259A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P260A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; S261A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;

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D262A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     V263A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
     K264A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y;
     N265A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 1266P;
     Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T274C;
     276A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; I277A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y;
     V280A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
     1283A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; S286P; S288P; *288aP, R289P;
     L293A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
10
     F294A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     W296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
     E297A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     P298A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     A299C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
15
     W300A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
     1301A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y;
     H302A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y:
     *302aA,C,D,E,F,G,H,1,K,L,M,N,P,Q,R,S,T,V,W,Y;
20
     *302dP; *302jA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302kA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302mA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302nA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *3020A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302qA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
25
     *302rA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302sA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302tA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302uA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
30
     *302vA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302xA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y,
     *302yA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302zA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302aaA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302bbA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302ccP;
35
     *302ddA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302eeA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *302ffA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
```

*302ggA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302hhA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302iiA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302jjA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N303A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; A304C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N305A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L306A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; G307A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 S308A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; \$309A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; C310A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A311C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y: D312A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 N313A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; T314A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; M315A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; F316A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S317A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; Q318A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; 20 S319A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; G320A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q321A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; A322C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L323A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S324P; S325P; 25 L326A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S327P; V328C;

F329A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; and/or Q330C.

The variant of any one of claims 1-3, wherein the variant comprises at least one of the following substitutions: G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 V7A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; D8A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 S9A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S10A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
 S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; V12A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
 V13A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V14A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
 E15A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E16A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 A18C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V20A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
 Y22A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N24P; T25P; A29P;
 L32A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L36A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;

N39C; T43A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; V44A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Q46A,C,D,E,F,G,H,1,K,L,M,N,P,R,S,T,V,W,Y; R47A,C,D,E,F,G,H,1,K,L,M,N,P,Q,S,T,V,W,Y; V48A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; W49A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; V50A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,,W,Y; N51A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 5 P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A53P; D54A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N56A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; Y57A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y61A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y77A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; D79A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F80A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 Y82A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S83A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; D84A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T85A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,,V,W,Y; W86A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; A87C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D88A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A90C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H91A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 Q92A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T93A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; M94A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; 95A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D101P; W107H,S; Y110C; Q126E; G133A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 20 E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 1136A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; R137A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;G139A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L140A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L141A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 25 W142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; T147P; W150C; G163C; H178A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L179A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D180A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N181A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 30 G182A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W183A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; D184A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W185A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; 35 G186A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T187A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; Q188A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;

N189A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N194C; Q198P; L203P; S204P;

G210A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; S212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; F213A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F216FVASTG; Y217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S218A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S219A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 10 S220A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; A221C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T222A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 15 S224A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; A225C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L226A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; K227A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; S228A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S229A.C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 20 L230A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D231A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N232A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; M233A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; 1241A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; 25 A242C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V244A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; N247A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; W248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; P249A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 1250A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; C252A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 35 P255A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; R256A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Y257A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;

\$258A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; F259A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P260A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; D262A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 5 V263A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T274C; F276A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 1277A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; V280A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 10 I283A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; S288P; L293A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; F294A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; W296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; 15 E297A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P298A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A299C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W300A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; I301A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 H302A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N303A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; A304C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N305A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L306A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 25 G307A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S308A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S309A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; C310A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A311C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 D312A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N313A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y: T314A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; M315A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; F316A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y: S317A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 35 Q318A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; \$319A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;

G320A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q321A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; A322P; S324P; S325P; L326A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S327P; V328C; F329A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; and/or Q330C.

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- 5. The variant of any one of claims 1-4, wherein the variant comprises at least one of the following substitutions:
- (a) Y214N,S+N247Y+L306Q; Y214A; F216FVASTG; and/or P89W+W86N;
- (b) A90S+H91D; H91N,L,D; N313D; N303D,H; and/or N305D,H;
- (c) Y22P, N24P, T25P, A29P, A53P, N56P, T93P, D101P, W142P, T147P, Q198P, L203P, S204P, S219P, S258P, S288P, A304P, A311P, Q318P, A322P, S324P, S325P, and/or S327P;
 - (d) W107S,H;
 - (e) Q126E;
- (f) N39C+L326C; V20C+G320C; Y110C+G163C; W150C+N194C; T274C+V328C; and/or I301C+F316C; and/or
 - (g) G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V7A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; D8A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W9A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; S10A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
- V12A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V13A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V14A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; E15A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E16A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

V20A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; Y22A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; L32A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L36A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;

- T43A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; V44A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Q46A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; ·
 - R47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; V48A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
 - W49A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; V50A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; N51A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
- 30 D54A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N56A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; Y57A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y61A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
 - Y77A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; D79A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - F80A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- Y82A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S83A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
 D84A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T85A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
 W86A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; A87C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - D88A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A90C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H91A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

Q92A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T93A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; M94A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; P95A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; G133A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 5 1136A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; R137A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; G139A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L140A,C,D.E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L141A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 10 W142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; H178A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L179A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D180A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 N181A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; G182A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W183A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; D184A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W185A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; G186A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 T187A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; Q188A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; N189A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; G210A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 25 S212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; F213A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 Y217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S218A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S219A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S220A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; A221C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 35 T222A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S224A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;

A225C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L226A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; K227A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; S228A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S229A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; L230A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D231A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y: N232A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; M233A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; 1241A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 A242C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y: V244A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; 15 N247A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; W248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; P249A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 1250A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; C252A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 P255A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; R256A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Y257A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S258A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; F259A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 25 P260A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; D262A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y: V263A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; 30 F276A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 1277A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; V280A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 1283A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; L293A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 35 F294A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; W296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; E297A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

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P298A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A299,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W300A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; 1301A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; H302A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 5 N303A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; A304C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N305A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L306A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 10 G307A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; \$308A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; \$309A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; C310A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A311C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D312A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 N313A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; T314A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; M315A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y: F316A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 S317A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; Q318A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; \$319A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; G320A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q321A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; L326A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; and/or 25 F329A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y,

6. The variant of any one of claims 3-5 which is a variant of a *Myceliophthora thermo-phila* galactanase.

7. The variant of any one of claims 1-2, wherein the variant comprises at least one of the following substitutions: *-6P; *-4P; *-2P; A1P; Q3P; K5A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D7A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W8A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; W9A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; V12A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; M13A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; V14A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; E15A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E16A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

- A18C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V20A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; Y22A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N24C,P; V25P; N26P; E29P; K30C; L32A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L36A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 39C; G40C; V41P; M43A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y;
- V44A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Q46A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; R47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; V48A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; W49A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; V50A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; N51A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
- W53A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 D54A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; *54aP;
 *54eA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 *54fA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 *54gA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- *54hA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 G55A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N56A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
 Y57A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N58A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
 Y61A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N62C; L65C; A69C;
 Y77A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N79A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
- F80A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y82A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S83A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; D84A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W86A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D88A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
- A90C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H91A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q92A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T93A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; T94A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; P95A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A96C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G97P; D101P; A106C; W107H,S; Y110C; T113C; L114C; Q126E; S131A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
- 30 G133A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; I136A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y;
- 35 G139A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L140A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L141A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; W142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; L144P;

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K146A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y;W142P; T147P; W150C; S159C; G163C;
      L169P; K172P; H178A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      L179A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
      D180A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      N181A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
      G182A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      W183A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
      N184A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
      W185A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
10
      D186A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      T187A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
      Q188A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;
      N189A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
      W191A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; N194C; Q198P; M203P; S204P;
      G210A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 15
      V211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
      S212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
      F213A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     Y214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
20
     F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 216FVASTG;
     Y217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     S218A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     A219C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     S220A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
25
     A221C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     T222A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
     L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
     D224A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     S225A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
30
     L226A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
     R227A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;
     R228A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;
     S229A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
35
     L230A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
     N231A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
     N232A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
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M233A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; V234C;
      V241A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
      A242C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
      V244A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
  5
      E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
      N247A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
      W248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
      P249A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
 10
      T250A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
      C252A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      *252dA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      *252eA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     P253A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
15
     Y254A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     P255A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     R256A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;
     Y257A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
20
     Q258A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;
     F259A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     P260A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     A261C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     D262A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     V263A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
25
     R264A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;
     N265A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; V266P;
     Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T274C;
     276A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; I277A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y;
     V280A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
30
     V283A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; S286P; S288P; *288aP; K289P;
     L293A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
     F294A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     W296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
35
     E297A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     P298A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
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A299C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

W300A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; I301A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; H302A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302aA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302dP; *302jA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302kA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302mA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302nA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *3020A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302qA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 *302rA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302sA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302tA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302uA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 *302vA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y: *302xA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y, *302yA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302zA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302aaA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 *302bbA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302ccP; *302ddA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302eeA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302ffA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302ggA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302hhA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 25 *302iiA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302jjA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N303A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y: A304C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 N305A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L306A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; G307A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S308A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S309A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; C310A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 35 A311C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D312A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y:

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N313A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y: T314A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; M315A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; F316A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T317A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y: P318A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; S319A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; G320A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q321A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;

- 10 A322C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L323A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S324P; S325P; L326A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S327P; V328C; F329A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; and/or H330C.
- 15 8. The variant of claim 7, wherein the variant comprises at least one of the following substitutions: G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V7A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D8A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W9A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; S10A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; V12A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; M13A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; V14A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 20 E15A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E16A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A18C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V20A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; Y22A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; V25P; E29P; L32A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L36A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 25 V41P; M43A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; V44A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Q46A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; R47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;
 - V48A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; W49A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; V50A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; N51A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
- W53A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D54A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; G55A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N56A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; Y57A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N58A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; Y61A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
- Y77A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N79A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 35 F80A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y82A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S83A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; D84A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T85A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;

W86A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; A87C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D88A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A90C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H91A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q92A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T93A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; T94A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; A96C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T113C; G133A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 1136A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 T137A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y: G139A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L140A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L141A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; W142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; G163C; L169P; H178A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 ·L179A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D180A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N181A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; G182A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W183A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; 20 N184A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; W185A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; D186A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T187A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; 25 Q188A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; N189A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; Q198P; M203P; G210A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; S212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; F213A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 Y214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 216FVASTG; Y217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S218A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 35 A219C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

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A221C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T222A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D224A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S225A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; L226A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; R227A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; R228A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; S229A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; L230A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 10 N231A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; N232A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; M233A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; V241A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; A242C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V244A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; N247A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;20 W248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; P249A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; C252A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P255A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; R256A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; 25 Y257A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Q258A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; F259A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P260A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A261P; D262A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 V263A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; Y276A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; 1277A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; V280A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V283A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; S288P; L293A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; F294A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; W296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; E297A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y: P298A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 5 A299C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y: W300A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; I301A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; H302A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y: N303A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; A304C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 N305A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L306A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; G307A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S308A,C,D,E,F,G,H,1,K,L,M,N,P,Q,R,T,V,W,Y; \$309A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 15 C310A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A311C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D312A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N313A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 20 T314A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; M315A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; F316A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T317A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; P318A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 25 S319A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; G320A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q321A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; A322P; S324P; S325P; L326A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; F329A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; and/or H330C.

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- 9. The variant of claim 8, wherein the variant comprises at least one of the following substitutions:
- (a) V20P, V25P, E29P, V41P, V50P, W53P, N56P, T94P, A96P, W142P, L169P, W185P, Q198P, M203P, A219P, A221P, T222P, Q258P, A261P, D262P, S288P, N305P, A311P, A322P, S324P, and/or S325P;
- (b) T113C+G163C, W185C+S229C, S218C+A221C, R227C+V283C; and/or
- (c) G6A,C,D,E,F,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; V7A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y;

. D8A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; W9A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,Y; \$10A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y; \$11A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y; 5 V12A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; M13A,C,D,E,F,G,H,I,J,K,L,N,P,Q,R,S,T,V,W,Y; V14A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; E15A,C,D,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; E16A,C,D,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 A18C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; V20A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; Y22A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W; L32A,C,D,E,F,G,H,I,J,K,M,N,P,Q,R,S,T,V,W,Y; L36A,C,D,E,F,G,H,I,J,K,M,N,P,Q,R,S,T,V,W,Y; 15 M43A,C,D,E,F,G,H,I,J,K,L,N,P,Q,R,S,T,V,W,Y; V44A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; R45A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,S,T,V,W,Y; Q46A,C,D,E,F,G;H,I,J,K,L,M,N,P,R,S,T,V,W,Y; R47A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,S,T,V,W,Y: 20 V48A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; W49A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,Y; V50A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; N51A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; P52A,C,D,E,F,G,H,I,J,K,L,M,N,Q,R,S,T,V,W,Y; W53A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,Y; 25 D54A,C,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; G55A,C,D,E,F,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; N56A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; Y57A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W; 30 N58A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; Y61A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W; Y77A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W; N79A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; F80A,C.D,E,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; 35 Y82A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W; \$83A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y;

D84A,C,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; T85A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,V,W,Y; W86A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,Y; A87C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; D88A,C,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; 5 P89A,C,D,E,F,G,H,I,J,K,L,M,N,Q,R,S,T,V,W,Y; A90C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; H91A,C,D,E,F,G,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; Q92A,C,D,E,F,G,H,I,J,K,L,M,N,P,R,S,T,V,W,Y; T93A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,V,W,Y; 10 T94A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,V,W,Y; A96,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; G133A,C,D,E,F,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; N134A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; E135A,C,D,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 I136A,C,D,E,F,G,H,J,K,L,M,N,P,Q,R,S,T,V,W,Y; T137A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,V,W,Y; G139A,C,D,E,F,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; L141A,C,D,E,F,G,H,I,J,K,M,N,P,Q,R,S,T,V,W,Y; W142A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,Y; 20 H178A,C,D,E,F,G,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; L179A,C,D,E,F,G,H,I,J,K,M,N,P,Q,R,S,T,V,W,Y; D180A,C,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; N181A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; G182A,C,D,E,F,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; 25 W183A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,Y; N184A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; W185A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,Y; D186A,C,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; T187A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,V,W,Y; 30 Q188A,C,D,E,F,G,H,I,J,K,L,M,N,P,R,S,T,V,W,Y; N189A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; G210A,C,D,E,F,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; V211A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; S212A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y; 35 F213A,C,D,E,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; Y214A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W; P215A,C,D,E,F,G,H,I,J,K,L,M,N,Q,R,S,T,V,W,Y;

F216A,C,D,E,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; Y217A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W; S218A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y; A219C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; S220A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y; A221C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; T222A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,V,W,Y; L223A,C,D,E,F,G,H,I,J,K,M,N,P,Q,R,S,T,V,W,Y; D224A,C,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 \$225A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y; L226A,C,D,E,F,G,H,I,J,K,M,N,P,Q,R,S,T,V,W,Y; R227A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,S,T,V,W,Y; R228A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,S,T,V,W,Y; \$229A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y; L230A,C,D,E,F,G,H,I,J,K,M,N,P,Q,R,S,T,V,W,Y; 15 N231A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; N232A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; M233A,C,D,E,F,G,H,I,J,K,L,N,P,Q,R,S,T,V,W,Y; V241A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; A242C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 V243A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; V244A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; E245A,C,D,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; T246A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,V,W,Y; 25 N247A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; W248A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,Y; P249A,C,D,E,F,G,H,I,J,K,L,M,N,Q,R,S,T,V,W,Y; C252A,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; P255A,C,D,E,F,G,H,I,J,K,L,M,N,Q,R,S,T,V,W,Y; R256A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,S,T,V,W,Y; 30 Y257A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W; Q258A,C,D,E,F,G,H,I,J,K,L,M,N,P,R,S,T,V,W,Y; F259A,C,D,E,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; P260A,C,D,E,F,G,H,I,J,K,L,M,N,Q,R,S,T,V,W,Y; D262A,C,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; . 35 V263A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; Q273A,C,D,E,F,G,H,I,J,K,L,M,N,P,R,S,T,V,W,Y; Y276A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W;

35

1277A,C,D,E,F,G,H,J,K,L,M,N,P,Q,R,S,T,V,W,Y; V280A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; V283A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,W,Y; L293A,C,D,E,F,G,H,I,J,K,M,N,P,Q,R,S,T,V,W,Y; 5 F294A,C,D,E,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y: Y295A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W; W296A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,Y; E297A,C,D,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; P298A,C,D,E,F,G,H,I,J,K,L,M,N,Q,R,S,T,V,W,Y; A299C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 W300A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,Y; 1301A,C,D,E,F,G,H,J,K,L,M,N,P,Q,R,S,T,V,W,Y; H302A,C,D,E,F,G,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; N303A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; A304C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 N305A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; L306A,C,D,E,F,G,H,I,J,K,M,N,P,Q,R,S,T,V,W,Y; G307A,C,D,E,F,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; S308A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y; S309A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y; 20 C310A,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; A311C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; D312A,C,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; N313A,C,D,E,F,G,H,I,J,K,L,M,P,Q,R,S,T,V,W,Y; T314A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,V,W,Y; 25 M315A,C,D,E,F,G,H,I,J,K,L,N,P,Q,R,S,T,V,W,Y; F316A,C,D,E,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; T317A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,S,V,W,Y; P318A,C,D,E,F,G,H,I,J,K,L,M,N,Q,R,S,T,V,W,Y; S319A,C,D,E,F,G,H,I,J,K,L,M,N,P,Q,R,T,V,W,Y; 30 G320A,C,D,E,F,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y; Q321A,C,D,E,F,G,H,I,J,K,L,M,N,P,R,S,T,V,W,Y; L326A,C,D,E,F,G,H,I,J,K,M,N,P,Q,R,S,T,V,W,Y; and/or F329A,C,D,E,G,H,I,J,K,L,M,N,P,Q,R,S,T,V,W,Y.

10. The variant of any one of claims 7-9 which is a variant of a *Humicola insolens* galactanase.

11. The variant of any one of claims 1-2, wherein the variant comprises at least one of the following substitutions: *-6P; *-4P; *-2P; A1P; T3P;

R5A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A7C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D8A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

- 5 I9A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; S10A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; L12A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L13A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L15A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
 - E16A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E18A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- Y20A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y22A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N24C,P; L25P; N26P; T29P; Q30C; A31P; L32A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L36A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; A39C; G40C; I41P;
 - S43A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; I44A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Q46A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;
- R47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; V48A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; W49A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; V50A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; N51A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; S53A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; D54A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *54aP; *54eA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- *54fA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 *54gA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 *54hA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - G55A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S56A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; Y57A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; D58A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- Y61A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N62C; L65C; V69C;
 Y77A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; D79A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 L80A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 L82A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S83A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
 D84A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T85A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
- 30 W86A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; A87,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D88A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; S90A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; D91A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q92A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T93A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; T94A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- S96A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; G97P; D101P; K106C; W107H,S; Y110C; T113C; L114C; D126E; G133A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

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I136A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y;
      R137A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;
      G139A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      L140A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
     L141A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
      W142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; L144P;
      E146A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T147P; Y150C; S159C; G163C; L169P;
      T171P; T172P; H178A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y;
      L179A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
      D180A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
10
      D181A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      G182A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
      W183A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
      $184A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     W185A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
15
      D186A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     Q187A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;
     Q188A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;
     N189A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
20
     F191A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T194C; T198P; E200P; S203P; T204P;
     G210A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     V211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
     S212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     Y213A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
25
     Y214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F216FVASTG;
     Y217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     S218A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     A219C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
30
     S220A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     A221C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     T222A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
     L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
35
     A224C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     S225A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     L226A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
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K227A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y;
     T228A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
     S229A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     L230A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
     A231C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 5
     N232A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y:
     L233A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; Q234C;
     V241A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y:
    V242A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
10
     V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y:
     V244A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
     E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
     N247A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
     W248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
    P249A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     V250A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
     C252A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     *252dA,C,D,E,F,G,H,1,K,L,M,N,P,Q,R,S,T,V,W,Y;
20
     *252eA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     P253A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     N254A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
     P255A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y:
     A256C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
25
     Y257A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W:
     A258C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     F259A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y:
     P260A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     S261A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
30
     D262A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     L263A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S264A,C,D,E,F,G,H,I,K,L,M,N,P,Q,T,V,W,Y;
     S265A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; I266P;
     Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; Q274C;
     F276A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y:
    L277A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
35
     L280A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
     V283A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; A286P; T288P; *288aP, D289P;
     V293A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
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Y294A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; W296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; E297A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P298A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 5 A299,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W300A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; I301A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; G302A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302aA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 *302dP; *302jA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302kA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302mA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302nA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *3020A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 *302qA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302rA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302sA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302tA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302uA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 *302vA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302xA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y, *302yA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302zA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302aaA,C,D,E,F,G,H,1,K,L,M,N,P,Q,R,S,T,V,W,Y; 25 *302bbA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302ccP; *302ddA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302eeA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302ffA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 *302ggA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302hhA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302iiA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *302jjA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N303A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; A304C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 35 G305A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L306A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;

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G307A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; \$308A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; \$309A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; C310A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A311C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D312A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N313A,C,D,E,F,G,H,I,K;L,M,P,Q,R,S,T,V,W,Y; L314A,C,D.E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; M315A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; V316A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 10 D317A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y318A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; T319A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; D320A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 E321A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V322A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; Y323A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; E324P; S325P; I326A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; E327P; T328C;

L329A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; and/or G330C.

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12. The variant of claim 11, wherein the variant comprises at least one of the following substitutions: T3P; R5A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A7C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D8A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; I9A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; S10A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 25 L12A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L13A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L14A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L15A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; E16A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E18A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y20A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y22A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; N24C,P; L25P; T29P; Q30C; A31P; L32A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 30 L36A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S43A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 144A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Q46A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; R47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; V48A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; W49A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; V50A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; N51A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 35 P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; S53P; D54A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D54A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; \$56A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; Y57A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;

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Y61A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; L65C;
     Y77A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; D79A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     L80A,C.D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     L82A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S83A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     D84A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T85A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
     W86A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; A87,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     D88A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     $90A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; D91A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     Q92A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T93A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
10
     T94A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; P95A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     S96P; G133A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
     E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     1136A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y;
15
     R137A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;
     G139A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     L141A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
     W142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; L144P; E146P; T147P; T172P;
     H178A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y;
     L179A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
20
     D180A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y:
     D181A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     G182A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     W183A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
25
     $184A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     W185A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
     D186A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     Q187A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;
     Q188A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;
30
     N189A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y:
     F191A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     E200P; S203P; G210A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     V211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y:
     $212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
35
     Y213A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     Y214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F216FVASTG:
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Y217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S218A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; A219C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S220A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; A221C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 5 T222A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; A224C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S225A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; L226A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 10 K227A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; T228A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; S229A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; L230A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;A231C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 N232A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L233A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; V242A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V244A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 20 E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;N247A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; W248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; P249A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 25 C252A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P255A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A256C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y257A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; A258C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 F259A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P260A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; S261P; D262A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L263A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S264P; I266P; Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; 35 F276A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L277A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L280A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;

V283A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; T288P; V293A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; Y294A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; W296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; E297A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P298A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A299,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W300A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; I301A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 G302A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y: N303A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; A304C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G305A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L306A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 15 G307A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S308A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S309A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; C310A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 A311C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D312A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N313A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L314A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; M315A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; 25 V316A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; D317A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y318A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; T319A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; D320A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 E321A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V322A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; Y323A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; E324P; S325P; I326A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; E327P; T328C; L329A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; and/or G330C.

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- 13. The variant of claim 12, wherein the variant comprises at least one of the following substitutions:
- (a) D181N, D181N+S90A+D91H;

- (b) T3P, Y20P, N24P, L25P, T29P, A31P, V50P, S53P, S56P, T93P, T94P, S96P, W142P, L144P, E146P, T147P, T172P, E200P, S203P, A219P, A256P, A258P, S261P, S264P, I266P, T288P, I301P, A304P, Y318P, and/or E324P;
- (c) L13C+L65C, N24C+Q30C, S218C+A221C, A304C+Y318C; and/or
- 5 (d) R5A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A7C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D8A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; I9A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; S10A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; L12A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L13A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
- L15A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; E16A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E18A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y22A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; L32A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L36A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L44A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;
- Q46A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; R47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; V48A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; V50A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N51A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; D54A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S56A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
- Y61A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y77A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; D79A.C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L80A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L82A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S83A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T85A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
- 25 A87C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D88A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; S90A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; D91A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q92A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T93A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; P95A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; G133A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
- 30 N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; I136A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; R137A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; G139A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 - L141A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; W142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; H178A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L179A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;

D180A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D181A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G182A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W183A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; \$184A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; W185A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; D186A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q187A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; Q188A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; 10 N189A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; G210A.C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; S212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; Y213A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; 15 Y214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S218A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 20 A219C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S220A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; A221C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T222A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 25 A224C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; \$225A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y: L226A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; K227A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; T228A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; S229A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 30 L230A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; A231C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N232A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L233A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 35 V242A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V244A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; N247A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; W248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; P249A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 5 C252A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y: P255A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A256C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y257A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; A258C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 F259A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P260A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; D262A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L263A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; 15 F276A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L277A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; L280A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; V283A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V293A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 20 Y294A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; W296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; E297A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P298A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 25 A2990C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W300A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; 1301A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; G302A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N303A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; A304C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 G305A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L306A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; G307A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; \$308A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S309A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; 35 C310A,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A311C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D312A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

N313A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
L314A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y;
M315A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y;
V316A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
D317A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
Y318A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
T319A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
D320A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
V322A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
I326A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
and/or
L329A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; and/or
(e) E18F,Y,W; L12V; L80F; L82Y; F191Y,W; Y213F; E18W+L12V; L82Y+L80F.

- 15 14. The variant of any one of claims 11-13 which is a variant of an Aspergillus aculeatus galactanase.
 - 15. The variant of any one of claims 1-2, wherein the variant comprises at least one of the following substitutions: K-6P; S-4P; L-2P; K1P; F3P;
- K5A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 V7A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; D8A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 V9A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; S10A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
 S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; I12A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y;
 I13A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; A14C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 L15A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; E16A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 S18A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; V20A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
 F22A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N24C,P; E25P; S26P; K29P; Q30C; D31P;
 - I32A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; L36A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; A39C; G40C; V41P; Y43A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
- V44A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;
 V46A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;
 I48A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; W49A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
 N50A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; D51A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; Y53A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
- D54A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A54aP;
 G54eA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y54fA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
 G54gA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 G54hA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

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G55A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N56A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; N57A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; D58A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; K61A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; A62C; I65C; A69C; L77A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D79A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F80A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y82A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D84A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F85A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W86A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D88A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A90C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; R92A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A94C,D,E,F

K96A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; A97P; N101P; K106C; T107H,S; Y110C;

T113C; K114C; D126E; Q131A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;
G133A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
T136A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
N137A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;

20 G139A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L140A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; A141C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *144P; G146A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E147P; W150C; A159C; A163C; *169P;

25 S171P; N172P; H178A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F179A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T180A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; N181A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;

30 E183A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
T184A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
S185A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
G186A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
R187A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;

P182A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;

Y188A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
 A189C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 I191A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; T194C; H198P; *200P; H203P; V204P;
 A210C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;



S211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; Y213A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W: P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F216FVASTG; W217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; *218A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *219A,C,D,E,F,G;H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 H220A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G221A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T222A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y: K224A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y: 15 N225A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L226A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; T227A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; S228A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; V229A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 20 L230A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; T231A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; S232A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; V233A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; A234C; V241A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 25 M242A,C,D,E,F,G,H,I,K,L,N,P,Q,R,S,T,V,W,Y; V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y: A244C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; 30 S247A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; Y248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; T249A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; Y250A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; A252C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D252dA,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 35 G252eA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

H253A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

G254A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N255A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; T256A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; A257C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P258A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; K259A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; N260A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; G261A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q262A.C.D.E.F.G.H.I.K.L.M,N,P,R,S,T,V,W,Y; T263A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; 10 L264A.C.D.E.F.G.H.I.K,M,N,P,Q,R,S,T,V,W,Y; N265A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; N266P; Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; A274C; A276C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V277A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 15 V280A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; A283C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D286P; G288P; E288aP, A289P; V293A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; F294A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; 20 W296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; E297A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P298A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A299C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W300A.C.D.E.F.G.H.I.K.L,M,N,P,Q,R,S,T,V,Y; 25 I301A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; P302A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; V302aA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; A302dP: N302iA,C,D,E,F,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 30 K302kA,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; L302mA,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; W302nA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; E302oA,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y302qA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; G302rA.C.D.E.F.H.I.K.L.M,N,P,Q,R,S,T,V,W,Y; 35 S302sA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; G302tA.C.D.E.F.H.I.K.L.M.N.P.Q.R.S.T.V.W.Y;

W302uA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;

A302vC,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T302xA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y. S302yA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y: Y302zA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; A302aaC,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A302bbC,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E302ccP; Y302ddA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; D302eeA,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P302ffA,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; 10 E302ggA,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D302hhA,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A302iiC,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y: G302jjA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; K303A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; 15 W304A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; F305A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G306A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G307A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S308A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y: 20 A309C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V310A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; D311A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N312A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y: Q313A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; 25 A314C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L315A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; F316A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D317A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F318A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; K319A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; 30 G320A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; R321A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; P322A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; L323A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; S325P; 35 L326A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; H327P; V328C;

F329A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; and/or Q330C.

The variant of claim 15, wherein the variant comprises at least one of the following 16. substitutions: K-6P; S-4P; L-2P; K1P; K5A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V7A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; D8A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V9A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; S10A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; A14C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L15A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; \$18C;V20P; \$26P; K29P; D31P; G40C; Y43A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; V44A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; V46A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; I48A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; W49A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; 10 N50A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; D51A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; Y53A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; A54aP; G54eA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y54fA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; G54gA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G54hA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G55A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 N56A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; N57A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; A62C; A69C; L77A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D79A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F80A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y82A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S83A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; D84A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 F85A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W86A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; A87C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D88A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A90C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; K91A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; Q92A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;K93A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; A94C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 25 P95A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A97P; N101P; K106C; K114C; Q131A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; G133A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 30 T136A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; N137A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; G139A.C.D.E.F.H.I.K.L.M.N.P.Q.R.S.T.V.W.Y; L140A.C.D.E.F.G.H.J.K.M.N.P.Q.R.S.T.V.W.Y; A141C.D.E.F.G.H.I.K.L.M.N,P,Q,R,S,T,V,W,Y; 35

*142A.C,D.E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *144P;

H178A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

G146A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A159C; A163C; S171P;

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F179A.C.D.E.G.H.I.K.L,M,N,P,Q,R,S,T,V,W,Y;
    T180A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
    N181A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
    P182A, C.D.E.F.G.H, I, K, L, M, N, Q, R, S, T, V, W, Y;
    E183A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
    T184A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; S185P;
     R187A.C.D.E.F.G.H.I.K.L.M.N.P.Q.S.T.V.W.Y;
     Y188A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     S211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     S212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
10
     Y213A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     Y214A, C, D, E, F, G, H, I, K, L, M, N, P, Q, R, S, T, V, W;
     P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
     F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F216FVASTG;
     W217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y;
15
     H220A.C.D.E.F.G.I.K.L.M.N.P.Q.R.S.T.V.W.Y;
     G221A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     T222A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y;
     L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
     N225A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
20
     L226A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
     T227C; A234C; V241C; V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;
     A244C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
25
     S247A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y;
     Y248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
     T249A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
     Y250C; D252dA,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
30
     G252eA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     H253A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     G254A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
     N255A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
     T256A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
     A257C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
35
     P258A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y;
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K259A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y;

N260A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; G261A,C.D.E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q262A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T263A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; L264A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; N265A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; N266P; Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; A276C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V277A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V280A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; A283C; D286P; E288aP; A289P; 10 V293A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; F294A, C, D, E, G, H, I, K, L, M, N, P, Q, R, S, T, V, W, Y; Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; W296A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; E297A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 15 P298A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; A299C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W300A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; 1301A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; V302aA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; A302dP; 20 N302jA,C,D,E,F,H,I,K,L,M,P,Q,R,S,T,V,W,Y; K302kA,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; L302mA,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; W302nA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; E3020A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 25 Y302qA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; G302rA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; S302sA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; G302tA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; W302uA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; 30 A302vC,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T302xA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y, \$302yA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; Y302zA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; A302aaC,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 35 A302bbC,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E302ccP; Y302ddA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; D302eeA,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

P302ffA,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; E302ggA,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D302hhA,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A302iiC,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G302jjA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; K303A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; W304A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; F305A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G306A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G307A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 10 S308A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; A309C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V310A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; D311A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N312A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; 15 Q313A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; A314C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L315A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; F316A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F318P; F329A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; and/or Q330C. 20

- 17. The variant of claim 16, wherein the variant comprises at least one of the following substitutions:
- (a) K-6P, S-4P, L-2P, K1P, V20P, S26P, K29P, D31P, A54aP, G54eP, N57P, K93P, A97P,
 N101P, S171P, S185P, T256P, N260P, N266P, D286P, E288aP, A289P, A302dP, S302yP,
 Y302zP, A302bbP, E302ccP, E302ggP, F305P, D311P, F318P;
 - (b) S18C+Y302qC, G40C+Q330C, V44C+A69C, I48C+A62C, N50C+D84C, G54gC+T302xC, N56C+G302rC, A62C+G146C, K106C+A159C, K114C+A163C, E183C+G221C, T227C+A283C, A234C+V241C, Y250C+Q273C, A302aaC+A302iiC; and/or
- (c) K5A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; G6A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V7A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; D8A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V9A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; S10A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; S11A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; L15A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; Y43A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; V44A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R45A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; V46A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; R47A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y;

P52A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; Y53A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; G54eA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y54fA,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; G54gA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G54hA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;

- G55A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N56A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; N57A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L77A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; D79A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F80A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H81A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y82A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; S83A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; D84A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; A87C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P89A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; K91A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; Q92A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; K93A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; P95A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P95A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; P95A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; P95A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;
- 15 P95A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; Q: G133A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N134A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; E135A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T136A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y;
- 20 N137A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
 G139A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 L140A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
 A141C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
 *142A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; *144P;
- 25 G146A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H178A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F179A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T180A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; N181A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
- 9182A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; E183A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T184A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; R187A,C,D,E,F,G,H,I,K,L,M,N,P,Q,S,T,V,W,Y; Y188A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;
 - 5 \$211A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; \$212A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; Y213A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; Y214A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;

P215A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; F216A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; F216FVASTG; W217A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,Y; H220A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G221A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 5 T222A,C,D,E,F,G,H,K,L,M,N,P,Q,R,S,T,V,W,Y; L223A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; N225A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; L226A,C.D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; V243A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 10 A244C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; E245A,C,D,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; T246A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; S247A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,T,V,W,Y; Y248A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W; 15 T249A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; Y250C; D252dA,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G252eA,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; H253A,C,D,E,F,G,I,K,L,M,N,P,Q,R,S,T,V,W,Y; G254A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; 20 N255A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; T256A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; A257C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; P258A,C,D,E,F,G,H,I,K,L,M,N,Q,R,S,T,V,W,Y; K259A,C,D,E,F,G,H,I,L,M,N,P,Q,R,S,T,V,W,Y; 25 N260A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; G261A,C,D,E,F,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Q262A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; T263A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,V,W,Y; L264A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y; 30 N265A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y; Q273A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y; A276C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; V277A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; V280A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; 35 V293A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y; F294A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y; Y295A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W;

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V310A,C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,W,Y;

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D311A,C,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
N312A,C,D,E,F,G,H,I,K,L,M,P,Q,R,S,T,V,W,Y;
Q313A,C,D,E,F,G,H,I,K,L,M,N,P,R,S,T,V,W,Y;
A314C,D,E,F,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
L315A,C,D,E,F,G,H,I,K,M,N,P,Q,R,S,T,V,W,Y;
F316A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y;
and/or
F329A,C,D,E,G,H,I,K,L,M,N,P,Q,R,S,T,V,W,Y.

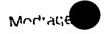
- 18. The variant of any one of claims 15-17 which is a variant of a *Bacillus licheniformis* galactanase.
 - 19. The variant of any one of claims 1-18, wherein the number designating each position is the number of the corresponding amino acid residue in SEQ ID NO: 1, said corresponding amino acid residue being derivable from an alignment according to Fig. 5 or 6, said alignment including the parent galactanase.
 - 20. The variant of any one of claims 1-19, wherein the parent galactanase has an amino acid sequence which has a degree of identity to the amino acid sequence of SEQ ID NO: 1 of at least 25%.
 - 21. The variant of any one of claims 1-20, wherein the parent galactanase is obtained from a strain of Yersinia, Aspergillus, Humicola, Meripilus, Myceliophthora, or Thermomyces., or from a strain of Bacillus, Bifidobacterium, Cellvibrio, Clostridium, Pseudomonas, Thermotoga, or Xanthomonas.
 - 22. An isolated nucleic acid sequence comprising a nucleic acid sequence which encodes the galactanase variant of any one of claims 1-21.
 - 23. A nucleic acid construct comprising the nucleic acid sequence of claim 22 operably
 30 linked to one or more control sequences that direct the production of the galactanase variant in a suitable expression host.
 - 24. A recombinant expression vector comprising the nucleic acid construct of claim 23.
 - 35 25. A recombinant host cell comprising the nucleic acid construct of claim 23 or the vector of claim 24.

- 26. A method for producing a galactanase variant of any one of claims 1-21, the method comprising (a) cultivating a recombinant host cell of claim 25; and (b) recovering the polypeptide.
- 5 27. Use of at least one galactanase variant of any one of claims 1-4 in the dairy industry.
 - 28. The use of claim 27 to prepare galacto-oligo-saccharides and/or for hydrolysis of lactose.

ABSTRACT

5

Variants of Glycoside Hydrolase family 53 galactanases, e.g. variants of the galactanases from strains of Yersinia, Aspergillus, Humicola, Meripilus, Myceliophthora, Thermomyces, Bacillus, Bifidobacterium, Cellvibrio, Clostridium, Pseudomonas, Thermotoga, or Xanthomonas.

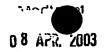


10319.010-DK

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10319.010-	DK				U O A	APR. ZUUJ	
			1/	174	-		
					t t	PVS	
HEADER						MTGL	MMCT
MOTA	1 CB ALA	1				1.00 29.91	MTGL MTGL
ATOM	2 C ALA	1	-			1.00 27.24	MTGL
ATOM	3 O ALA	1		-2.394		1.00 27.44 1.00 29.26	MTGL
ATOM	4 N ALA	1		-5.006			MTGL
ATOM	5 CA ALA	1		-3.540		1.00 28.32 1.00 25.13	MTGL
ATOM	6 N LEU	2		-3.378	19.034 19.486	1.00 23.13	MTGL
ATOM	7 CA LEU	2		-2.955 -3.322	20.957	1.00 23.07	MTGL
MOTA	8 CB LEU	2		-3.322 -2.507		1.00 23.57	MTGL
MOTA	9 CG LEU	2		-3.090	23.384	1.00 23.95	MTGL
MOTA	10 CD1 LEU	2		-1.057	21.940	1.00 23.31	MTGL
MOTA	11 CD2 LEU	2		-3.574	18.664	1.00 22.07	MTGL
MOTA	12 C LEU	2		-4.757	18.340	1.00 21.83	MTGL
ATOM	13 O LEU 14 N THR	2 3		-2.767	18.329	1.00 20.29	MTGL
ATOM		3		-3.257	17.575	1.00 19.63	MTGL
MOTA	15 CA THR 16 CB THR	3	23.506	-2.100	16.978	1.00 20.33	MTGL
ATOM	17 OG1 THR	3		-1.360	16.083	1.00 20.92	MTGL
ATOM ATOM	18 CG2 THR	3 3 3	24.728	-2,626	16.227	1.00 20.96	MTGL
MOTA	19 C THR	3	23.610	-4.038	18.515	1.00 19.16	MTGL
ATOM	20 O THR	3	24.131	-5.092	18.156	1.00 19.29	MTGL MTGL
ATOM	21 N TYR	4	23.796	-3.514	19.724	1.00 18.09	MTGL
ATOM	22 CA TYR	4	24.652	-4.159	20.715	1.00 17.42 1.00 17.15	MTGL
MOTA	23 CB TYR	4	25.724	-3.180	21.202	1.00 17.13	MTGL
ATOM	24 CG TYR	4	26.514	-2.544	20.082	1.00 17.43	MTGL
MOTA	25 CD1 TYR	4	27.516	-3.251	19.412 18.348	1.00 17.43	MTGL
MOTA	26 CE1 TYR	4	28.210	-2.678	19.661	1.00 17.07	MTGL
MOTA	27 CD2 TYR	4	26.229	-1.246 -0.666	18.598	1.00 18.55	MTGL
ATOM	28 CE2 TYR	4	26.916 27.902	-1.386	17.948	1.00 17.59	MTGL
MOTA	29 CZ TYR	4	28.564	-0.814	16.891	1.00 18.07	MTGL
ATOM	30 OH TYR 31 C TYR	4 4	23.858	-4.657	21.912	1.00 16.29	MTGL
ATOM	31 C TYR 32 O TYR	4	23.210	-3.876	22.615	1.00 16.95	MTGL
ATOM	33 N ARG	5	23.907	-5.964	22.125	1.00 15.87	MTGL
ATOM ATOM	34 CA ARG	5	23.232	-6.611	23.244	1.00 16.37	MTGL
ATOM	35 CB ARG	5	22.281	-7.711	22.746	1.00 17.04	MTGL
ATOM	36 CG ARG	5	21.203	-7.235	21.764	1.00 18.21	MTGL MTGL
ATOM	37 CD ARG	5	20.189	-8.348	21.482	1.00 18.30	MTGL
MOTA	38 NE ARG	5	20.839	-9.547	20.950	1.00 19.36 1.00 20.62	MTGL
ATOM	39 CZ ARG	5	21.243	-9.681	19.692	1.00 20.62	MTGL
MOTA	40 NH1 ARG	5	21.054	-8.696		1.00 19.43	MTGL
ATOM	41 NH2 ARG	5		-10.790	19.307 24.009	1.00 16.18	MTGL
MOTA	42 C ARG	5	24.390 24.869	-7.238 -8.311		1.00 16.58	MTGL
ATOM	43 O ARG	5	24.853	-6.577		1.00 16.16	MTGL
MOTA	44 N GLY	6	25.991	-7.135		1.00 16.79	MTGL
ATOM	45 CA GLY	6 6	26.064	-7.065		1.00 15.64	MTGL
ATOM	46 C GLY 47 O GLY	6	25.129	-6.664		1.00 15.46	MTGL
ATOM	47 O GLY 48 N VAL	7	27.213	-7.497		1.00 15.87	MTGL
ATOM	49 CA VAL	7	27.491	-7.500	29.199	1.00 15.12	MTGL
ATOM ATOM	50 CB VAL	ż	27.178	-8.877	29.846	1.00 14.43	MTGL
ATOM	51 CG1 VAL	7	25.750	-9.293	29.537	1.00 12.85	MTGL
ATOM	52 CG2 VAL	7	28.170	-9.931	29.348	1.00 13.29	MTGL
MOTA	53 C VAL	7	28.977	-7.238	29.363	1.00 16.14	MTGL MTGL
ATOM	54 O VAL	7	29.768	~7.469		1.00 17.27	MTGL
MOTA	55 N ASP	8	29.354	-6.737		1.00 15.62 1.00 15.20	MTGL
ATOM	56 CA ASP	8	30.755	-6.514			MTGL
MOTA	57 CB ASP	В	30.920	-5.292	2 31.751	7.00 14.33	

Fig. 1



10319.010	-DK		0/474	PVS	PVS	
			2/174			
's most	58 CG ASP	8	32.373 -4.975	32.034 1.00 15.24	MTGL	
ATOM	58 CG ASP 59 OD1 ASP	8	33.105 -5.881	32.486 1.00 14.12	MTGL	
ATOM ATOM	60 OD2 ASP	8	32.784 -3.817	31.805 1.00 14.89	MTGL	
ATOM	61 C ASP	8	31.108 -7.793	31.602 1.00 14.33	MTGL	
ATOM	62 O ASP	8	30.573 -8.040	32.683 1.00 15.61	MTGL	
ATOM	63 N TRP	9	31.980 -8.614	31.027 1.00 13.27	MTGL	
ATOM	64 CA TRP	9	32.365 -9.872	31.653 1.00 13.40	MTGL	
ATOM	65 CB TRP	9	32.124 -11.020	30.663 1.00 12.58	MTGL MTGL	
ATOM	66 CG TRP	9	33.183 -11.146	29.585 1.00 13.96	MTGL	
ATOM	67 CD2 TRP	9	33.682 -12.362	29.012 1.00 13.39 28.057 1.00 13.29	MTGL	
ATOM	68 CE2 TRP.	9	34.661 -12.008		MTGL	
MOTA	69 CE3 TRP	9	33.396 -13.719		MTGL	
ATOM	70 CD1 TRP	9	33.860 -10.128	28.964 1.00 14.11 28.046 1.00 13.31	MTGL	
MOTA	71 NE1 TRP	9	34.752 -10.640 35.357 -12.964	27.305 1.00 14.73	MTGI.	
ATOM	72 CZ2 TRP	9	34.093 -14.673	28.463 1.00 14.84	MTGL	
MOTA	73 CZ3 TRP	9 9	35.059 -14.287	27.523 1.00 14.12	MTGL	
MOTA	74 CH2 TRP 75 C TRP	9	33.832 -9.860	32.102 1.00 13.91	MTGL	
ATOM	75 C TRP 76 O TRP	9	34.454 -10.915	32.272 1.00 13.71	MTGL	
MOTA MOTA	77 N SER	10	34.373 -8.660	32.295 1.00 13.08	MTGL	
ATOM	78 CA SER	10	35.770 -8.481	32.692 1.00 14.15	MTGL	
ATOM	79 CB SER	10	35.983 -7.052	33.193 1.00 13.75	MTGL	
ATOM	80 OG SER	10	35.691 -6.114	32.168 1.00 14.07	MTGL	
MOTA	81 C SER	.10	36.321 -9.460	33.726 1.00 14.36	MTGL MTGL	
ATOM	82 O SER	10	37.414 -9.994	33.553 1.00 14.45 34.789 1.00 14.45	MTGL	
ATOM	83 N SER	11	35.561 -9.697		MTGL	
MOTA	84 CA SER	11	35.985 -10.588	35.870 1.00 15.55 37.069 1.00 15.32	MTGL	
MOTA	85 CB SER	11	35.053 -10.416 33.795 -11.014	36.792 1.00 13.85	MTGL	
MOTA	86 OG SER	11	36.043 -12.080	35.544 1.00 16.02	MTGL	
ATOM	87 C SER	11	36.438 -12.870	36.401 1.00 16.91	MTGL	
ATOM	88 O SER 89 N VAL	11 12	35.656 -12.472	34.330 1.00 16.04	MTGL	
ATOM	89 N VAL 90 CA VAL	12	35.640 -13.890	33.969 1.00 14.89	MTGL	
ATOM ATOM	91 CB VAL	12	35.367 -14.090	32.448 1.00 14.61	MTGL	
ATOM	92 CG1 VAL	12	36.418 -13.371	31.604 1.00 13.79	MTGL	
MOTA	93 CG2 VAL	12	35.336 -15.583	32.124 1.00 13.78	MTGL	
ATOM	94 C VAL	12	36.861 -14.726	34.373 1.00 15.76	MTGL MTGL	
ATOM	95 O VAL	12	36.709 -15.751	35.034 1.00 14.51 33.990 1.00 16.87	MTGL	
ATOM	96 N VAL	13	38.065 -14.312		MTGL	
MOTA	97 CA VAL	13	39.246 -15.100	34.343 1.00 17.35 33.534 1.00 17.20	MTGL	
MOTA	98 CB VAL	13	40.496 -14.656 41.775 -15.198	34.177 1.00 16.12	MTGL	
ATOM	99 CG1 VAL	13	40.391 -15.193		MTGL	
MOTA	100 CG2 VAL 101 C VAL	13 13	39.534 -15.043	35,841 1.00 18.53	MTGL	
ATOM	101 C VAL 102 O VAL	13	40.002 -16.024	36.430 1.00 19.44	MTGL	
MOTA MOTA	103 N VAL	14	39.242 -13.907	36.466 1.00 17.79	MTGL	
ATOM	104 CA VAL	14	39.463 -13.785	37.900 1.00 18.35	MTGL	
MOTA	105 CB VAL	14	39.106 -12.368	38.411 1.00 18.68	MTGL	
ATOM	106 CG1 VAL	14	39,117 -12.347		MTGL	
ATOM	107 CG2 VAL	14	40.113 -11.352		MTGL MTGL	
ATOM	108 C VAL	14	38.588 -14.816		MTGL	
ATOM	109 O VAL	14	39.034 -15.495		MTGL	
MOTA	110 N GLU	15	37.341 -14.941		MTGL	
ATOM	111 CA GLU	15	36.420 -15.889		MTGL	
ATOM	112 CB GLU	15	34.985 -15.585 34.392 -14.361		MTGL	
ATOM	113 CG GLU	15	34.392 -14.301	· · · · · · · · · · · · · · · · · · ·	MTGL	
ATOM	114 CD GLU 115 OE1 GLU	15 15	35.113 -14.887		MTGL	
MOTA	115 OE1 GLU	1.3	33.223 2.100	- 		

Fig. 1 cont.

	070 010	15	32.984 -14.445 40.981 1.00 22.28	MTGL
ATOM	116 OE2 GLU	15	36 753 _17 346 3B.502 1.00 18.41	MTGL
atom	117 C GLU	15	36 640 -18 196 39,377 1.00 19.29	MTGL
ATOM	118 O GLU		37 151 -17 639 37.272 1.00 18.79	MTGL
MOTA	119 N GLU	16	37 504 -19 006 36,921 1.00 19.07	MTGL
ATOM	120 CA GLU	16	37.827 -19.103 35.424 1.00 19.33	MTGL
MOTA	121 CB GLU	16	36.645 -18.735 34.530 1.00 19.54	MTGL
MOTA	135 CG GFR	16	30.043 10	MTGL
ATOM	123 CD GLU	16	30.970 -10.730 30	MTGL
MOTA	124 OE1 GLU	16	30.173	MTGL
MOTA	125 OE2 GLU	16	30.040 23.0.0	MTGL
MOTA	126 C GLU	16	30.700 #2	MTGL
ATOM	127 O GLU	16	30.700 20.30	MTGL
ATOM	128 N ARG	17	33.040 20125	MTGL
ATOM	129 CA ARG	17	40.042 40.00	MTGL
MOTA	130 CB ARG	17	41.0/2 4.1	MTGL
MOTA	131 CG ARG	17	42.000	MTGL
ATOM	132 CD ARG	17	40.440 10.12	MTGL
MOTA	133 NE ARG	17	44.246 -16.636 35.801 1.00 15.36	MTGL
ATOM	134 CZ ARG	17	45.084 -15.708 35.357 1.00 15.76	MTGL
ATOM	135 NH1 ARG	17	45.225 -14.570 36.025 1.00 15.62	MTGL
MOTA	136 NH2 ARG	17	45.788 -15.922 34.254 1.00 15.66	
ATOM	137 C ARG	17	40.502 -18.887 40.225 1.00 18.97	MTGL
ATOM	138 O ARG	17	41.279 -19.407 41.017 1.00 19.60	MTGL
MOTA	139 N ALA	18	39.330 -18.396 40.590 1.00 19.85	MTGL
ATOM	140 CA ALA	18	38.890 -18.486 41.967 1.00 21.00	MTGL
	141 CB ALA	18	38.071 -17.262 42.339 1.00 21.45	MTGL
MOTA	142 C ALA	18	39 066 -19 756 42 154 1.00 21 · ¹ 8	MTGL
MOTA	143 O ALA	18	37.495 -19.982 43.216 1.00 21.53	MTGL
ATOM	144 N GLY	19	37 994 -20.577 41 110 1.00 20.78	MTGL
ATOM	145 CA GLY	19 .	37 265 -21.827 41.218 1.00 21.14	MTGL
MOTA	146 C GLY	19	35.833 -21.845 40.716 1.00 21.86	MTGL
MOTA	147 O GLY	19	35.124 -22.833 40.901 1.00 20.92	MIGL
ATOM	148 N VAL	20	35 386 -20 769 40.080 1.00 21.60	MTGL
ATOM	149 CA VAL	20	34.021 -20.755 39.578 1.00 21.91	MTGL
ATOM	150 CB VAL	20	33 533 -19 321 39.264 1.00 23.06	MTGL
MOTA	151 CG1 VAL	20	32 126 -19 370 38.674 1.00 22.39	MTGL
ATOM	152 CG2 VAL	20	33 530 -18 475 40.530 1.00 22.53	MTGL
MOTA	153 C VAL	20	33 877 -21 589 38,305 1.00 21.53	MTGL
MOTA	154 O VAL	20	34 673 -21 473 37.377 1.00 21.65	MTGL
MOTA		21	32 864 -22 444 38 283 0.50 21.24	MTGL
ATOM		21	32 596 -23 272 37.116 0.50 21.35	MTGL
MOTA		21	32 602 -24 757 37.488 0.50 22.01	MTGL
MOTA		21	33 897 -25 165 37.901 0.50 22.69	MTGL
ATOM	158 OG SER 159 C SER	21	31 227 -22.857 36.605 0.50 20.74	MTGL
ATOM		21	30 205 -23 167 37.214 0.50 20.32	MTGL
MOTA		22	31 216 -22 134 35.491 1.00 20.34	MTGL
ATOM		22	29 972 -21,659 34,914 1.00 20.72	MTGL
ATOM		22	30 270 -20 511 33.952 1.00 19.18	MTGL
ATOM		22	30 765 -19 280 34.682 1.00 18.50	MTGL
MOTA	164 CG TYR 165 CD1 TYR	22	29 909 -18.548 35,503 1.00 17.85	MTGL
MOTA		22	30 357 -17 428 36.202 1.00 17.95	MTGL
MOTA	166 CE1 TYR 167 CD2 TYR	22	32 092 -18 865 34.578 1.00 17.87	MTGL
MOTA		22	32 552 -17 744 35,275 1.00 17.81	MTGL
MOTA	168 CE2 TYR	22	31 676 -17.031 36.083 1.00 17.46	MTGL
ATOM	169 CZ TYR	22	32 107 -15 915 36.767 1.00 17.47	MTGL
MOTA	170 OH TYR		29 152 -22.742 34.239 1.00 21.41	MTGL
ATOM	171 C TYR	22	29 688 -23 634 33.588 1.00 21.91	MTGL
ATOM	172 O TYR	22	27.839 -22.654 34.414 1.00 22.66	MTGL
MOTA	173 N LYS	23	211000 221001 21110	

Fig. 1 cont.

	_			00	26.918 -23.619 33.836 1.00 23.97	MTGL
MOTA	174		LYS	23	26.387 -24.537 34.936 1.00 24.47	MTGL
MOTA	175		LYS	23	27.479 -25.094 35.839 1.00 26.17	MTGL
ATOM	176	CG	LYS	23	26.894 -25.778 37.066 1.00 28.12	MTGL
MOTA	177	CD	LYS	23	27.985 -26.217 38.040 1.00 29.23	MTGL
MOTA	178	CE	LYS	23	28.750 -25.069 38.615 1.00 28.37	MTGL
MOTA	179	NZ	LYS	23	25.748 -22.915 33.158 1.00 24.07	MTGL
ATOM	180	Ç	LYS	23	25.344 -21.823 33.570 1.00 23.42	\mathtt{MTGL}
ATOM	181	0	LYS	23	25.210 -23.557 32.125 1.00 25.34	MTGL
MOTA	182	N	ASN	24	24.074 -23.020 31.390 1.00 26.76	MTGL
ATOM	183	CA	ASN	24	23.907 -23.741 30.042 1.00 27.22	MTGL
MOTA	184	CB	ASN	24	23.925 -25.258 30.174 1.00 28.00	MTGL
ATOM	185	CG	ASN	24	23.925 -25.250 50.2.	MTGL
MOTA	186		ASN	24	23.300 23.000 ==	MTGL
MOTA	187	ND2	ASN	24	24.020 23.020	MTGL
MOTA	188	C	ASN	24		MTGL
ATOM	189	0	ASN	24	22,000	MTGL
MOTA	190	N	THR	25	21.031 00.000	MTGL
MOTA	191	CA	THR	25	20.400 221.01	MTGL
ATOM	192	CB	THR	25	13,23	MTGL
MOTA	193	OG1	THR	25	13,203 04,044 =	MTGL
ATOM	194	CG2	THR	25	13,000 +00.00	MTGL
ATOM	195	С	THR	25	13.300 2.122	MTGL
ATOM -	196	0	THR	25	13-10, 210-0	MTGL
ATOM	197	N	ASN	26	20.301 20.700	MTGL
MOTA	198	CA	ASN	26	20.223	MTGL
ATOM	199	CB	ASN	26		MTGL
ATOM	200	CG	ASN	26	19,010 21.11.	MTGL
MOTA	201		. ASN	26		MTGL
ATOM	202	ND2	ASN	26	10.525 20.525	MTGL
MOTA	203	С	ASN	26	21.000	MTGL
ATOM	204	0	ASN	26	40.104	MTGL
MOTA	205	N	GLY	27	21,002 20,100	MTGL
ATOM	206	CA	GLY	27	22,,07 20,320	MTGL
MOTA	207	С	GLҮ	27	24.000	MTGL
MOTA	208	0	GLY	27	24,002	MTGL
ATOM	209	N	ASN	28	24,000	MTGL
MOTA	210	CA	NZA	28		MTGL
ATOM	211	ĊВ	ASN	28	20.020	MTGL
ATOM	212	ÇG	ASN	28	21,010	MTGL
ATOM	213	OD:	1 ASN	28	24.400	MTGL
ATOM	214	ND	2 ASN	28		MTGL
ATOM	215	С	ASN	28	20,714 27,220 02,	MTGL
ATOM	216	0	ASN	28	20.337 20.000	MTGL
MOTA	217	N	ALA	29	2/102/ 2:102	MTGL
ATOM	218	CA		29	27.100 20.002	MTGL
ATOM	219	CB		29	30.230 27.00	MTGL
ATOM	220	C	ALA	29		MTGL
MOTA	221	. 0	ALA	29	251252	MTGL
MOTA	222		GLN	30		MTGL
ATOM	223		GLN	30	29.967 -24.655 29.603 1.00 23.10 28.620 -24.424 28.901 1.00 23.68	MTGL
MOTA	224		GLN	30	201020	MTGL
ATOM	225			30	28.676 -23.687 27.578 1.00 26.45	MTGL
ATOM	226			30	27.335 -23.695 26.858 1.00 27.43	MTGL
ATOM	-227	OE	1 GLN	30	26.282 -23.584 27.486 1.00 27.66	MTGL
ATOM	228		2 GLN	30	27.371 -23.815 25.537 1.00 27.00	MIGL
ATOM	229		GLN	30	30.748 -23.350 29.740 1.00 21.50	MTGL
ATOM	230		GLN	30	30.556 -22.609 30.700 1.00 21.61	MTGL
ATOM	231		PRO	31	31.661 -23.066 28.797 1.00 20.08	HIGH
		-				

Fig. 1 cont.

·			222	21	.32.110 -23.	886	27.657	1.00	20.60	\mathtt{MTGL}
MOTA	232	-	PRO	31 31	32.432 -21.		28.886	1.00	19.48	MTGL
ATOM	233	-	PRO		33.262 -21.		27.603	1.00	20.47	MTGL
ATOM	234	-	PRO	31	33.489 -23.	309	27.369		20.52	MTGL
ATOM	235	CG	PRO	31	31.492 -20.		28.960		18.32	MTGL
ATOM	236	C	PRO	31	30.491 -20		28.246	1.00	17.02	MTGL
MOTA	237	0	PRO	31	31.811 -19	664	29.828		18.30	MTGL
ATOM	238		LEU	32	30.971 -18	477	29.987	1.00	18.52	MTGL
MOTA	239		LEU	32	31.623 -17	476	30.954	1.00	17.22	MTGL
MOTA	240		LEU	32	30.828 -16	190	31.227	1.00	17.71	MTGL
MOTA	241	CG	LEU	32	29,443 -16	536	31.767		15.78	MTGL
MOTA	242	CD1		32	31.588 -15	310	32.235	1.00	15.40	MTGL
ATOM	243	CD2		32	30.655 ~17	776	28.669	1.00	17.46	MTGL
MOTA	244	C	LEU	32	29.504 -17	412	28.429	1.00	18.85	\mathtt{MTGL}
MOTA	245	0	LEU	32	31.660 ~17	501	27.818	1.00	16.99	MTGL
ATOM	246	N	GLU	33			26.546		17.55	MTGL
ATOM	247	CA	GLU	33	31.421 -16		25.735		17,22	MTGL
MOTA	248	CB	GLU	33	32.716 -16	, / 0 3	25.424		16.64	MTGL
MOTA	249	CG	GLU	33	33.426 -18	.0//	26.453		16.72	MTGL
MOTA	250	CD	GLU	33	34.496 -18		27.667		14.95	MTGL
ATOM	251		GLU	33	34.234 -18	.2/0	26.048		16.02	MTGL
ATOM	252	OE 2	GLU	33	35.597 -18	. 640	25.712	1 00	18.39	MTGL
MOTA	253	С	GLU	33	30.369 -17			1 00	19.97	· MTGL
ATOM	254	Ò	GLU	33	29.576 -16	. 988	25.021 25.779	1.00	18.00	MTGL
ATOM	255	N	ASN	34	30.354 -18	3.959	25.779	1.00	19.90	MTGL
ATOM	256	CA	ASN	34	29.381 -19	0.739			21.66	MTGL
ATOM	257	CB	ASN	34	29.793 -21		24.955		24.08	MTGL
MOTA	258	CG	ASN	34	31.121 -21	.420	24.251	1.00	25.77	MTGL
ATOM	259	OD1	ASN	34	31.355 -20).886	23.168		26.27	MTGL
MOTA	260	ND2	ASN	. 34	31.995 -22	2.207	24.861		19.84	MTGL
ATOM	261	С	ASN	34	27.991 -19		25.640		19.75	MTGL
ATOM	262	0	ASN	34	26.988 -19		24.931		18.73	MTGL
MOTA	263	N	ILE	35	27.932 -19		26.967		18.63	MTGL
ATOM	264	CA	ILE	35	26.656 -19		27.656		18.28	MTGL
ATOM	265	CB	ILE	35	26.845 -19	9.440	29.188	1.00	17.35	MTGL
MOTA	266		ILE	35	25.556 -19	3.028	29.890		18.06	MTGL
MOTA	267		ILE	35	27.270 -20		29.623		19.14	MTGL
MOTA	268	CD1	ILE	35	27.652 -20		31.091	1.00	18.92	MTGL
MOTA	269	С	ILE	35	26.048 -18		27.258		18.51	MTGL
MOTA	270	0	ILE	35	24.867 -1		26.907		18.03	MTGL
MOTA	271	N	LEU	36	26.866 -1	7.005	27.313	1.00	17.16	MTGL
ATOM	272	CA	LEU	36	26.416 -1	5.665	26.956	1.00	17.06	MTGL
ATOM	273	CB	LEU	36	27.563 -1		27.110		16.94	MTGL
ATOM	274	CG	LEU	36	28.076 -1	4.411	28.538		14.36	MTGL
ATOM	275	CD1	LEU	36	29.323 -1	3.516	28.504		0 16.43	MTGL
MOTA	276	CD2	LEU	36	26.969 -1		29.372			MTGL
MOTA	277	С	LEU	36	25.891 -1		25.522		0 17.26	MTGL
ATOM	278	0	TEU	36	24.795 -1	5.132	25.270		0 16.08	MTGL
MOTA	279	N	ALA	37	26.675 -1	6.174	24.569		0 17.12	MTGL
ATOM	. 280	CA	ALA	37	26.278 -1	6.203			0 17.86	MTGL
ATOM	281	СВ	ALA	37	27.362 -1	6.863	22.338	1.0	0 16.93	MTGL
ATOM	282	С	ALA	37	24.961 -1		23.014		0 18.20	
ATOM	283	0	ALA	37	24.062 -1		22.314		0 19.46	MTGL
MOTA	284	N	ALA	38	24.850 -1	8.105	23.658		0 18.38	MTGL
ATOM	285		ALA	38	23.643 -1	8.917	23.560		0 20.05	MTGL
ATOM	286		ALA		23.809 -2	0.212	24.358		0 19.05	MTGL
ATOM	287		ALA		22.419 -1	.8,154	24.049		0 20.48	MTGL
ATOM	288		ALA		21.294 -1	.8.447	23.634		0 21.25	MTGL
ATOM	289		ASN		22.637 -1	7.173	24.923	1.0	0 20.10	MTGL
W+O1.1	200	••			- marin					

Fig. 1 cont.

		7.511	39	21.531 -	16 390	25.460	1.00 19.15	MTGL
MOTA		CA ASN	39	21.717 -		26.963	1.00 19.77	MTGL
MOTA	291	CB ASN		21.416 -			1.00 19.60	MTGL
MOTA	292	CG ASN	39	22.241 -			1.00 22.00	MTGL
MOTA	293	OD1 ASN		20.224 -		28.346	1.00 18.25	MTGL
MOTA	294	ND2 ASN		21.253 -		24.768	1.00 18.64	MTGL
ATOM	295	C ASN		20.544 ~		25.317	1.00 19.42	MTGL
MOTA	296	O ASN		20.544 ~		23.572	1.00 17.47	MTGL
MOTA	297	N GLY		21.803 -		22.837	1.00 17.26	MTGL
MOTA	298	CA GLY		21.535 -		22.880	1.00 17.22	MTGL
ATOM	299	C GLY		22.585 -	11 504	22.095	1.00 17.12	MTGL
MOTA	300	O GLY		22.523 -			1.00 16.80	MTGL
MOTA	301	N VAL		23.544 -		23.791	1.00 15.92	MTGL
MOTA	302	CA VAI		24.589 -	11.631	23.893	1.00 15.32	MTGL
MOTA	303	CB VAI	. 41	25.510 -		25.103	1.00 14.75	MTGL
MOTA	304	CG1 VA1		26.630 -	-10.888	25.144	1.00 14.75	MTGL
ATOM	305	CG2 VAI	, 41	24.707 -		26.397	1.00 15.77	MTGL
MOTA	306	C VAI	41	25.441 -		22.626		MTGL
ATOM	307	O VAI	41	25.832 -		22.158	1.00 14.76	MTGL
ATOM	308	N ASI	1 42	25.724 -		22.064	1.00 16.34	MTGL
ATOM	309	CA ASN	1 42	26.559 -		20.864	1.00 16.57	MTGL
ATOM	310	CB ASI	1 42	25.771	-9.889	19.646	1.00 17.06	MTGL
ATOM	311	CG ASI	v 42	25.299	-8.443	19.798	1.00 18.15	MTGL
ATOM	312	OD1 ASI	v 42	25.727	-7.709	20.694	1.00 18.63	
MOTA	313	ND2 ASI	42	24.416	-8.028	18.898	1.00 16.75	MTGL
ATOM	314	C ASI		27.812	-9.560	21.048	1.00 16.81	MTGL
MOTA	315	O ASI		28.651	-9.478	20.147	1.00 17.52	MTGL
ATOM	316	N TH		27.952	-8.951	22.221	1.00 16.55	MTGL
MOTA	317	CA TH		29.108	-8.108	22.502	1.00 15.96	MTGL
ATOM	318	CB TH		28.827	-6.634	22.136	1.00 16.50	MTGL
ATOM	319	OG1 TH		28.192	-6.565	20.850	1.00 17.26	MTGL
ATOM	320	CG2 TH		30.123	-5.840	22.102	1.00 15.22	MTGL
ATOM	321	C TH		29.487	-8.144	23.976	1.00 15.93	MTGL
ATOM	322	O TH		28.618	-8.180	24.849	1.00 16.10	MTGL
MOTA	323	N VA		30.786	-8.148	24.251	1.00 14.74	MTGL
ATOM	324	CA VA		31.251	-8.136	25.626	1.00 15.41	MTGL
ATOM	325	CB VA		32.038	-9.418	26.012	1.00 16.13	MTGL
MOTA	326	CG1 VA			-10.603	26.096	1.00 16.11	MTGL
ATOM	327	CG2 VA		33,146	-9.689	25.004	1.00 14.58	MTGL
MOTA	328	C VA	_ : .	32.137	-6.922	25.849	1.00 15.69	MTGL
	329	O VA		32.974	-6.574	25.014	1.00 16.22	MTGL
MOTA	330	N AR		31.916	-6.271	26.981	1.00 14.86	MTGL
MOTA	331	CA AR	_	32,662	-5.091	27.383	1.00 15.51	MTGL
MOTA	332	CB AF		31.702	-4.129	28.087	1.00 16.51	MTGL
MOTA	333	CG AF		32.297	-2.828	28.597	1.00 17.41	MTGL
MOTA	334	CD AF		31.143	-1.971	29.107	1.00 18.63	MTGL
MOTA	335	NE AF	· · ·	31.519	-0.636	29.554	1.00 19.44	MTGL
ATOM		CZ AF		31.756	-0.309	30.820	1.00 19.56	MTGL
ATOM	336	NH1 AF		31,671	-1.225	31.777	1.00 18,15	MTGL
MOTA	337			32.032	0.949			MTGL
ATOM	338	NH2 AF		33.752	-5.561	28.342	1.00 15.10	MTGL
MOTA	- 339			33,516	-6.446			MTGL
MOTA	340		RG 45	34.938	-4.965			MTGL
MOTA	341		LN 46	36.071	-5.331	29.074		MTGL
ATOM	342		LN 46	37.030	-6.246			MTGL
ATOM	343		LN 46	36.376	-7.512			MTGL
ATOM	344		LN 46		-8.358			MTGL
ATOM	345		LN 46	37.310				MTGL
MOTA	346			36.895	-9.363			MTGL
ATOM	347	NE2 G	LN 46	38.575	-7.958	20.014	1.00 10.24	

Fig. 1 cont.

•		_	C7 13	16	36.831	~4.089	29.534	1.00 15.79	MTGL
MOTA	348	_	GLN	46 46	37.153	-3.211	28.728	1.00 15.74	MTGL
MOTA	349	-	GLN	47	37.111	-4.005	30.830	1.00 15.01	MTGL
ATOM	350		ARG	47	37.851	-2.866	31.350	1.00 15.05	MTGL
ATOM	351		ARG	47	37.524	-2.631	32.828	1.00 13.91	MTGL
ATOM	352		ARG	47	37.649	-3.868	33.710	1.00 13.56	MTGL
ATOM	353	-	ARG	47	37.391	-3.520	35.175	1.00 13.26	MTGL
ATOM	354		ARG	47	37.207	-4.710	36.004	1.00 12.49	MTGL
MOTA	355	NE	ARG ARG	47	36.063	-5.382	36.117	1.00 13.71	MTGL
MOTA	356	CZ NH1		47	34.983	-4.981	35.457	1.00 13.79	MTGL
ATOM	357	NH2		47	36.004	-6.477	36.876	1.00 12.61	MTGL
ATOM	358		ARG	47	39.347	-3.107	31.182	1.00 15.50	MTGL
ATOM	359 360	С 0	ARG	47	39.849	-4.209	31.433	1.00 15.21	MTGL
ATOM	361	N	VAL	48	40.056	-2.072	30.745	1.00 15.84	MTGL
ATOM	362	CA	VAL	48	41,496	-2.171	30.557	1.00 15.53	MTGL
MOTA MOTA	363	CB	VAL	48	41.899	-1.874	29.102	1.00 16.38	MTGL
ATOM	364	CG1		48	43.418	-1.906	28.975	1.00 15.45	MTGL
ATOM	365		VAL	48	41.258	-2.892	28.160	1.00 14.39	MTGL
ATOM	366	C	VAL	48	42.222	-1.185	31.459	1.00 16.31	MTGL
ATOM	367	ŏ	VAL	48	41.941	0.013	31.433	1.00 14.76	MTGL
ATOM	368	N	TRP	49	43.139	-1.707	32.270	1.00 16.64	MTGL
ATOM	369	CA	TRP	49	43.938	-0.890	33.172	1.00 17.13	MTGL
MOTA	370	CB	TRP	49	43.893	-1.458	34.598	1.00 17.19	MTGL
MOTA	371	CG	TRP	49	42.525	-1.365	35.239	1.00 17.50	MTGL MTGL
ATOM	372	CD2		49	42.129	-1.903	36.510	1.00 17.36	MTGL
MOTA	373	CE2	TRP	49	40.773	-1.550	36.710	1.00 17.08	MTGL
ATOM	374	CE3	TRP	49	42.786	-2.651	37.497	1.00 16.24 1.00 17.53	· MTGL
ATOM	375	CD1	TRP	49	41.426	-0.728	34.736	1.00 17.33	MTGL
ATOM	376	NE1	TRP	49	40.370	-0.832	35.614	1.00 17.76 1.00 16.34	MTGL
ATOM	377	CZ2		49	40.063	-1.915	37.860	1.00 18.34	MTGL
ATOM	378	CZ3		49	42.079	-3.014	38.642	1.00 17.30	MTGL
ATOM	379	CH2		49	40.729	-2.645	38.812 32.632	1.00 17.96	MTGL
ATOM	380	С	TRP	49	45.369	-0.870	32.032	1.00 16.92	MTGL
ATOM	381	0	TRP	49	45.819	-1.830 0.228	32.874	1.00 18.74	MTGL
MOTA	382	N	VAL	50	• 46.078	0.408	32.373	1.00 18.43	MTGL
MOTA	383	CA	VAL	50	47.438 47.898	1.865	32.604	1,00 17.51	MTGL
ATOM	384	CB	VAL	50	49.310	2.061	32.069	1.00 16.69	MTGL
ATOM	385		VAL	50	49.310	2.814	31.912	1.00 16.38	MTGL
MOTA	386		VAL	50 50	48.492	-0.568	32.910	1.00 20.17	MTGL
MOTA	387	C	VAL	50	49.035	-1.359	32.141	1.00 20.17	MTGL
MOTA	388	О И	VAL ASN	51	48.809	-0.513	34.203	1.00 20.54	MTGL
ATOM	389 390	CA	ASN	51	49.800	-1.438	34:780	1.00 22.14	MTGL
MOTA MOTA	391	CB	ASN	51	51.181	-0.778	34.894	1.00 22.82	MTGL
ATOM	392	ÇĞ	ASN	51	51.899	-0.671	33.564	1.00 24.64	MTGL
ATOM	393		L ASN	51	52.211	0.430	33.102	1.00 25.29	MTGL
ATOM	394		2 ASN	51	52,180	-1.813		1.00 24.48	MTGL
ATOM	395		ASN	51	49.416	-1.943	36.173	1.00 22.18	MTGL
ATOM	396		ASN	51	50.177			1.00 23.10	MTGL
ATOM	397		PRO	52	48.242	-2.5B4		1.00 21.49	MTGL
ATOM	398		PRO	52	47.333	-3.089			MTGL
ATOM	399			52	47.847				MTGL MTGL
ATOM	400		PRO	52	46.509				MTGL
MOTA	401		PRO	52	46.683				MTGL
ATOM	402		PRO	52	48.905				MTGL
MOTA	403		PRO	52	49.390				MTGL
ATOM	404	N	ALA		49.261			1.00 22.20	MTGL
MOTA	405	CA	ALA	53	50.278	-4.739	40.061	1.00 23.49	MIGD

Fig. 1 cont.

ATOM	406	CB F	ALA	53	50.409	-4.407	41.549	1.00 23.83	MTGL .
ATOM	407	C P	LA	53	50.037	-6.235	39.883	1.00 23.68	MTGL
ATOM	408	O 7	ALA	53	50.937	-6.960	39.466	1.00 23.33	MTGL
MOTA	409	N P	ASP	54	48.831	-6.704	40.195	1.00 24.06	MTGL
ATOM	410	CA A	ASP	54	48.539	-8.126	40.058	1.00 24.64	MTGL MTGL
ATOM	411	CB A	ASP	54	47.400	-8:540	40.994	1.00 26.42	
ATOM	412	CG A	ASP	54	46.109	-7.805	40.706	1.00 27.54	MTGL MTGL
ATOM	413	OD1 A	ASP	54	45.834	-7.515	39.522	1.00 29.32	MTGL
ATOM	414	OD2 7	ASP	54	45.360	-7.529	41.664	1.00 27.59	
ATOM	415	C I	ASP	54	48.207	-8.560	38,631	1.00 24.00	MTGL MTGL
ATOM	416	0 1	ASP	54	47.878	-9.720	38.396	1.00 24.44	
MOTA	417	N (GLY	55	48.286	-7.630	37.686	1.00 22.74	MTGL
ATOM	418	CA (GLY	55	48.013	-7.959	36.296	1.00 21.74	MTGL
MOTA	419	C	GLY	55	46.566	-8.102	35.854	1.00 20.84	MTGL
ATOM	420	0	GLY	55	46.294	-8.150	34.652	1.00 20.70	MTGL
MOTA	421	N :	ASN	56	45.627	-8.173	36.791	1.00 20.23	MTGL
ATOM	422	CA	ASN	56	44.229	-8.320	36.399	1.00 19.77	MTGL
ATOM	423	CB .	ASN	56	43.329	-8.530	37.623	1.00 21.09	MTGL
ATOM	424	CG .	ASN	56	43.569	-9.876	38.301	1.00 22.81	MTGL
ATOM	425	OD1	ASN	56	43.921		37.647	1.00 20.74	MTGL MTGL
ATOM	426	ND2	ASN	56	43.359	-9.926	39.611	1.00 22.17	MTGL
MOTA	427	C	ASN	56	43.751	-7.108	35.612	1.00 18.30	MTGL
ATOM	428	0	ASN	56	43.972	-5.968	36.016	1.00 17.82	MTGL
MOTA	429	N	TYR	57	43.108	-7.376	34.480	1.00 16.29	MTGL
ATOM	430	CA	TYR	57	42.570	-6.353	33.591	1.00 15.51	MTGL
ATOM	431	CB	TYR	57	41.680	-5.376	34.368	1.00 15.50	MTGL
MOTA	432	CG	TYR	57	40.756	-6.062	35.348	1.00 16.25 1.00 15.93	MTGL
ATOM	433	CD1		57	39.969	-7.150	34.955	1.00 15.93	MTGL
MOTA	434	CE1		57	39.137	-7.799	35.859	1.00 16.23	MTGL
ATOM	435	CD2		57	40.681	-5.642	36.671	1.00 17.00	MTGL
MOTA	436	CE2		57	39.847	-6.288	37.585	1.00 17.00	MTGL
MOTA	437	CZ	TYR	57	39.080	-7.363	37.172 38.066	1.00 15.12	MTGL
MOTA	438	OH	TYR	57	38.254	-8.000	32.807	1.00 15.53	MTGL
MOTA	439	C	TYR	57	43.627	-5.579	32.189	1.00 14.98	MTGL
MOTA	440	0	TYR	57 50	43.315	-4.561 -6.033	32.825	1.00 14.46	MTGL
MOTA	441	N	ASN	58	44.877	-5.327	32.032	1.00 15.65	MTGL
ATOM	442	CA	ASN	58	45.876	-5.594	32.522	1.00 15.44	MTGL
ATOM	443	CB	ASN	58	47.314 47.783	-7.030	32.319	1.00 16.49	MTGL .
ATOM	444	CG	ASN	58		-7.390	32.779	1.00 18.71	MTGL
ATOM	445	OD1		58	48.869 46.995	-7.844	31.640	1.00 13.70	MTGL
ATOM	446	ND2		58 58	45.660	-5.763	30.582	1.00 16.00	MTGL
ATOM	447	C	ASN	58	44.774	-6.579	30.317	1.00 14.12	MTGL
ATOM	448	0	ASN LEU	59	46.447	-5.235	29.649	1.00 16.39	MTGL
MOTA	449	N	LEU	59	46.241	~5.564	28.242	1.00 17.31	MTGL
ATOM	450 451	CA CB	LEU	59 59	47.192	-4.751	27.356	1.00 17.07	MTGL
MOTA	452	CG	LEU	59	46.797	-4.743	25.874	1.00 17.21	MTGL
MOTA				59	45.367	-4.208	25.722	1.00 16.29	MTGL
ATOM	453 454		LEU	59	47.769	-3.882	25.085	1.00 16.17	MTGL
ATOM	455	C	LEU	59	46.333	-7.046	27.880	1.00 17.51	MTGL
ATOM	456	Ö	LEU	59	45.517	-7.537	27.096	1.00 17.20	MTGL
ATOM ATOM	457	й	ASP	60	47.317	-7,754	28.432		MTGL
ATOM	458	CA	ASP	60	47.460	-9.183	28.152	1.00 18.05	MTGL
ATOM	459		ASP	60	48.700	-9.768		1.00 20.82	MTGL
ATOM	460	CG	ASP	60	49.995			1.00 23.01	MTGL
ATOM	461		ASP	60	50.012			1.00 25.11	MTGL
ATOM	462		ASP	60	51.002			1.00 25.50	MTGI.
ATOM	463		ASP	60	46.237			1.00 17.40	MTGL
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Fig. 1 cont.

n mon	464	^	ASP	60	45.749 -10.856 27.984	1.00 16.59	MTGL
MOTA	464 465		TYR	61	45.756 -9.573 29.827	1.00 15.42	MTGL
MOTA	465	CA	TYR	61	44.580 ~10.215 30.398	1.00 15.67	\mathtt{MTGL}
MOTA	467		TYR	61	44.266 -9.581 31.759	1.00 15.24	MTGL
ATOM	46B	CG	TYR	61	43.000 -10.071 32.427	1.00 15.21	MTGL
MOTA	469		TYR	61	41.746 -9.597 32.032	1.00 15.96	MTGL
MOTA	470		TYR	61	40.578 -10.025 32.670	1.00 14.87	MTGL
ATOM	471		TYR	61	43.058 -10.990 33.473	1.00 15.54	MTGL
MOTA	472	CE2	TYR	61	41.899 -11.428 34.120	1.00 14.46	MTGL
MOTA	473	CZ	TYR	61	40.662 -10.943 33.714	1.00 16.75	MTGL
ATOM ATOM	474	OH	TYR	61	39.511 -11.379 34.345	1.00 14.25	MTGL
ATOM	475	C	TYR	61	43,400 -10.042 29.434	1.00 15.36	MTGL
ATOM	476	Ö	TYR	61	42.651 -10.987 29.175	1.00 15.76	MTGL
MOTA	477	N	ASN	62	43.257 -8.834 28.897	1.00 14.42	MTGL
MOTA	478	CA	ASN	62	42.174 -8.509 27.971	1.00 16.00	MTGL
MOTA	479	CB	ASN	62	42.072 -6.990 27.811	1.00 15.99	MTGL
ATOM	480	CG	ASN	62	41.231 -6.354 28.895		MTGL
ATOM	481		ASN	62	39,998 -6,396 28.840	1.00 18.23	MTGL
ATOM	482		ASN	62	41.887 ~5.780 29.901		MTGL
ATOM	483	Ç	ASN	62	42.306 -9.172 26.600		MTGL
MOTA	484	ŏ	ASN	62	41.306 -9.546 25.990		MTGL
ATOM	485	N	ILE	63	43.534 -9.311 26.110	1.00 16.06	MTGL
ATOM	486	CA	ILE	63	43.732 ~9.952 24.824	1.00 17.20	MTGL
ATOM	487	CB	ILE	63	45.202 -9.827 24.350		MTGL
ATOM	488		ILE	63	45.481 -10.814 23.214	1.00 17.67	MTGL
ATOM	489		ILE	63	45.463 -8.391 23.887		MTGL
ATOM	490		ILE	63	46.910 -8.105 23.521		MTGL
ATOM	. 491	С	ILE	63	43.333 -11.420 24.945		MTGL
ATOM	492	0	ILE	63	42.664 -11.964 24.068		MTGL
ATOM	493	N	ALA	64	43.722 -12.058 26.046	1.00 17.70	MTGL
MOTA	494	CA	ALA	64	43.379 -13.463 26.253		MTGL
ATOM	495	CB	ALA	64	44.000 -13.971 27.555		MTGL
ATOM	496	C	ALA	64	41.860 -13.703 26.262		MTGL
ATOM	497	0	ALA	64	41.370 -14.616 25.599	1.00 17.31	MTGL MTGL
MOTA	498	N	ILE	65	41.104 -12.895 27.002		MTGL
MOTA	499	CA	ILE	65	39.665 -13.117 27.030		MTGL
ATOM	500	CB	ILE	65	38.991 -12.503 28.289		MTGL
MOTA	501		ILE	65	39.574 -13.130 29.53		MTGL
MOTA	502	CG1		65	39.173 -10.984 28.323 38.423 -10.321 29.47		MTGL
ATOM	503		ILE	65			MTGL
MOTA	504	C	ILE	65			MTGL
MOTA	505	0	ILE	65 66	37.938 -13.101 25.36 39.598 -11.609 25.10		MTGL
ATOM	506	N	ALA	66	39.036 -11.087 23.86		MTGL
MOTA	507	CA	ALA	66 66	39.806 -9.854 23.40		MTGL
MOTA	508	CB	ALA		39.106 -12.185 22.80		MTGL
MOTA	509	C	ALA	66 66	38.189 -12.330 21.98		MTGL
ATOM	510	0	ALA	67	40.188 -12.965 22.81		MTGL
ATOM	511	N	LYS		40.340 -14.059 21.85		MTGL
ATOM	512	CA	LYS	67 67	41.700 -14.748 22.01		MTGL
MOTA	513	CB	LYS LYS	67	42.892 -13.953 21.48	4 1.00 23.60	MTGL
MOTA	514 515	CG	LYS	67	44.159 -14.795 21.55		MTGL
ATOM	516	CE	LYS	67	45.365 -14.050 21.00	0 1.00 29.59	MTGL
ATOM ATOM	517	NZ	LYS	67	45.208 -13.714 19.55		MTGL
ATOM	518	C	LYS	67	39.229 -15.085 22.07	0 1.00 19.44	MTGL
ATOM	519	Ö	LYS	67	38.667 -15.616 21.10		MTGL
ATOM	520	N	ARG	68	38.921 -15.365 23.33	5 1.00 18.94	MTGL
ATOM	521	CA	ARG		37.866 -16.317 23.67	2 1.00 17.61	MTGL
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Fig. 1 cont.

ATOM	522	CB	ARG	68	37.834 -	16.567	25.181	1.00	16.99	MTGL
				68	38.950 -	7 488	25.679	1.00	18.79	MTGL
ATOM	523	CG	ARG		39.015 -	17 515	27.199	1 00	17.89	MTGL
MOTA	524	CD	ARG	68	39.013 -	17.515	27.809		18.08	MTGL
ATOM	525	NE	ARG	68	37.742 -					
ATOM	526	CZ	ARG	68	37.555 -		29.120		18.59	MTGL
MOTA	527	NH1	ARG	68	38.561 -	17.798	29.961		18.68	MTGL
ATOM	528	NH2	ARG	68	36.371 -		29.595	1.00	16.96	MTGL
	529		ARG	68	36.511 -		23.209	1.00	17.25	MTGL
ATOM		C			35.679 ~		22.711		15.99	MTGL
ATOM	530	0	ARG	68			23.395		16.95	MTGL
ATOM	531	N .	ALA	69	36.285 -				18.21	MTGL
MOTA	532	CA	ALA	69	35.030 -		22.982			
ATOM	533	CB	ALA	69	·35.001 -		23.393		18.02	MTGL
MOTA	534	С	ALA	69	34.907 -	14.012	21.465		18.17	MTGL
ATOM	535	0	ALA	69	33.867 -	14.407	20.945		16.83	MTGL
ATOM	536	N	LYS	70	35.984 ~		20.764	1.00	18.35	MTGL
			LYS	70	36.011 -		19.312		19.84	MTGL
ATOM	537	CA			37,402 -		18.795		19.40	MTGL
ATOM	538	CB	LYS	70					21.56	MTGL
MOTA	539	CG	LYS	70	37.548 -		17.284		22.53	MTGL
ATOM	540	CD	LYS	70	38.992 -		16.892			
ATOM	541	CE	LYS	70	39.180 -	13.123	15.383		23.66	MTGL
MOTA	542	NZ	LYS	70	40.592 -	12.852	15.015		21.95	MTGL
ATOM	543	C	LYS	70	35.648 -	15.186	18.861	1.00	20.29	MTGL
ATOM	544	ŏ	LYS	70	34.842 -		17.948	1.00	19.93	MTGL
	545	N	ALA	71	36.235 -		19.511	1.00	19.37	MTGL
ATOM				71	35,970 -		19.159		20.95	MTGL
ATOM	546	CA	ALA				19.941		20.90	MTGL
MOTA	547	CB	ALA	71	36.896 -				21.38	MTGL
ATOM	548	С	ALA	71		17.975	19.405			MTGL
ATOM	549	0	ALA	71	34.010 -		18.810		22.34	
ATOM	550	N	ALA	72	33.839 ~	17.244	20.282		20.63	MTGL
ATOM	551	CA	ALA	72	32.439 -	-17.529	20.574	1.00	20.92	MTGL
MOTA	552	CB	ALA	72	32,149 -	17.284	22.050		20.20	MTGL
ATOM	553	č	ALA	72	31.523 -		19.710	1.00	20.68	MTGL
ATOM	554	ŏ	ALA	72	30.305 -		19.899		20.23	MTGL
				73	32.116 -		18.768		20.42	MTGL
MOTA	555	N	GLY		31,339 -		17.889		20.87	MTGL
MOTA	556	CA	GLY	73					21.42	MTGL
MOTA	557	С	GLY	73	30.874 -		18.523		21.96	MTGL
ATOM	558	0	GLY	73	29.946 -		18.027			
ATOM	559	N	LEU	74	31.522 -		19.612		20.70	MTGL
ATOM	560	CA	LEU	74	31.160 -	-12.146	20.315		19.98	MTGL
ATOM	561	CB	LEU	74	31.221 -	-12.372	21.830	1.00	19.61	MTGL
MOTA	562	CG	LEU	74	30.359	-13.491	22,420	1.00	19.97	MTGL
ATOM	563		LEU	74	30.692		23.898	1,00	19.32	MTGL
			LEU	74	28.881		22.232	1.00	18.79	MTGL
ATOM	564			74	32.071		19.960		19.91	MTGL
MOTA	565	C	LEU		33.292		19.882	1.00		MTGL
MOTA	566	0	LEU	74					19.06	MTGL
MOTA	567	И	GLY	75	31.473	-9.809	19.740			MTGL
ATOM	56B	CA	GLY	75	32.261	-8.627	19.438		18.36	
ATOM	569	C	GLY	75	32.856	-8.106	20.738		17.17	MTGL
ATOM	570	0	GLY	75	32.380	-8.457	21.821	1.00	16.83	MTGL
ATOM	571	N	VAL	76	33.885	-7.271	20.648	1.00	16.99	MTGL
ATOM	572	CA	VAL	76	34.522	-6.748	21,853		17.15	MTGL
	573	CB	VAL	76	35.996	-7.202	21.947		18.28	MTGL
ATOM			VAL		36.626	-6.682	23.238	1.00	17.92	MTGL
ATOM	574			76 76		-8.726	21.896	1 00	17.32	MTGL
ATOM	575		VAL	76	36.074				17.67	MTGL
MOTA	576	С	VAL	76	34.476	-5.231	21.984			MTGL
MOTA	577	0	VAL	76	34.770	~4.491	21.039		18.33	
ATOM	578	N	TYR	77	34.108	-4.785	23.177		16.77	MTGL
ATOM	579	CA	TYR	77	34.013	-3.366	23.517	1.00	16.63	MTGL

Fig. 1 cont.

	500	OD !	nVD	77	32.608	~3,102		1.00 15.27	MTGL
ATOM	580		TYR	רֹל	32.335	-1.799	24.840	1.00 15.55	MTGL
MOTA	581		TYR	77	33.343	-0.886	25.149	1.00 15.39	MTGL
ATOM	582		TYR	77	33.068	0.257	25.925	1.00 16.48	MTGL
MOTA	583	_	TYR	77	31.046	-1.532	25.312	1.00 16.02	MTGL
ATOM	584		TYR TYR -	, , , לל	30.766	-0.414	26.075	1.00 15.87	MTGL
ATOM	585			77	31.772	0.475	26.386	1.00 16.20	MTGL
MOTA	586		TYR	77	31.471	1,541	27.200	1.00 15.93	MTGL
ATOM	587		TYR	לי, לל	35.114	-3.128	24.548	1.00 16.00	MTGL
ATOM	588	-	TYR	77	35.026	-3.604	25.683	1.00 16.53	MTGL
ATOM	589		TYR	78	36.163	-2.419	24.142	1.00 16.29	MTGL
ATOM	590		ILE	78 78	37.280	-2.121	25.044	1.00 17.09	MTGL
ATOM	591		ILE	78 78	38.611	-2.008	24.261	1.00 17.14	MTGL
ATOM	592		ILE	78	39.695	-1.387	25.140	1.00 16.04	MTGL
MOTA	593	_		78	39.049	-3.394	23.777	1.00 16.84	MTGL
MOTA	594		ILE	78 78	39.424	-4.364	24.905	1.00 17.38	MTGL
MOTA	595		ILE	78	37.031	-0.818	25.818	1.00 17.27	MTGL
ATOM	596	С	ILE	78	36.834	0.241	25.227	1.00 17.22	MTGL
ATOM	597	0		79	37.046	-0.912	27.142	1.00 16.43	MTGL
MOTA	598	N	ASP ASP	79	36.817	0.234	28.009	1.00 16.05	MTGL
MOTA	599	CA	ASP	79	35.738	-0.127	29.039	1.00 17.34	MTGL
MOTA	600	CB	ASP	79	35,577	0.920	30.133	1.00 19.18	. MTGL
ATOM	601	CG OD1		79	36.023	2.072	29.952	1.00 19.88	MTGL
ATOM	602			79	34.986	0.583	31.181	1.00 20.19	\mathtt{MTGL}
MOTA	603	OD2	ASP	79	38.113	0.657	28.699	1.00 16.01	MTGL
MOTA	604	C	ASP	79 79	38.479	0.102	29.732	1.00 15.54	MTGL
MOTA	605	0	PHE	80	38.810	1.626	28.105	1.00 15.57	MTGL
ATOM	606	N	PHE	80	40.065	2.138	28.654	1.00 15.49	MTGL
MOTA	607	CA CB	PHE	80	40.811	3.005	27.627	1.00 14.72	MTGL
MOTA	608		PHE	80	41.533	2.230	26.566	1.00 14.70	MTGL
ATOM	609	CG CD1	PHE	80	42.548	1.343	26.899	1.00 14.82	MTGL
ATOM	610		PHE	80	41.224	2.419	25.222	1.00 15.80	MTGL
MOTA	611 612		PHE	80	43.251	0.649	25.912	1.00 15.54	MTGL
ATOM	613		PHE	80	41.921	1.730	24.221	1.00 16.06	MTGL
MOTA	614	CEZ	PHE	80	42.938	0.844	24.568	1.00 14.92	MTGL
ATOM ATOM	. 615	C	PHE	80	39.800	3.009	29.869	1.00 16.16	MTGL
ATOM	616	ŏ	PHE	80	39.126	4.036	29.759	1.00 15.79	MTGL
ATOM	617	N	HIS	81	40.328	2.617	31.025	1.00 15.76	MTGL
	618	CA	HIS	81	40.140	3.419	32.234	1.00 15.04	MTGL
MOTA MOTA	619	CB	HIS	81	40.130	2.533	33.485	1.00 13.87	MTGL
ATOM	620	CG	HIS	81	38.846	1.790	33.686	1.00 14.70	MTGL
ATOM	621		HIS	81	37.971	1,263	32.795	1.00 13.78	MTGL
ATOM	622		HIS	81	38.312	1.554	34.933	1.00 13.45	MTGL
ATOM	623		HIS	81	37.161	0.918	34.804	1.00 15.90	MTGL
ATOM	624		HIS	81	36.931	0.730	33.516	1.00 14.78	MTGL
ATOM	625	C	HIS	81	41.244	4.466	32.357	1.00 15.46	MTGL
ATOM	626	õ	HIS	81	41.113	5.439	33.102	1.00 14.94	MTGL
ATOM	627	N	TYR	82	42.326	4.273	31.609	1.00 15.09	MTGL
ATOM	628		TYR		43.452	5.199	31.663		MTGL
ATOM	629		TYR		43.092	6.520		1.00 15.74	MTGL
MOTA	630		TYR		42.849		29.476		MTGL
ATOM	631	CD1	TYR		43.702		28.680		MTGL
ATOM	632		TYR		43.527		27.307		MTGL
ATOM	633		TYR		41.801				MTGL
ATOM	634				41.613		27.465	1.00 16.11	MTGL
MOTA	635		TYR		42.482		26.705		MTGL
ATOM	636		TYR		42.331	6.148	25.345		MTGL
ATOM	637		TYR		43.866		33.122	1.00 17.11	MTGL
MION	557	•	• •						

Fig. 1 cont.

		_	mvn	02	43.987	6.573	33.593	1.00 17.37	MTGL
ATOM	638		TYR	82 83	44.077	4.329		1.00 17.17	MTGL
MOTA	639	N	SER	83	44.482	4.328	35.223	1.00 17.21	MTGL
MOTA	640	CA	SER SER	83	43.288	4.679	36.115	1.00 16.41	MTGL
ATOM	641	CB	SER	83	43.639	4.651	37.487	1.00 16.64	MTGL
ATOM	642	OG	SER	83	44.948	2.904	35.518	1.00 17.88	MTGL
ATOM	643	C	SER	83	44.689	1.993	34.732	1.00 17.59	MTGL
ATOM	644	0	ASP	84	45.646	2.706	36.630	1.00 18.00	MTGL
ATOM	645	N	ASP	84	46.106	1.369	36.984	1.00 17.91	MTGL
MOTA	646	CA	ASP	84	47.378	1.415	37.840	1.00 18.31	MTGL
ATOM	647	CB	ASP	84	48.570	1.993	37.105	1.00 19.40	MTGL
MOTA	648 649	CG OD1		84	48.732	1.724	35.897	1.00 18.50	MTGL
ATOM	650	OD2		84	49.366	2.705	37.750	1.00 20.89	MTGL
ATOM ATOM	651	C	ASP	84	45.017	0.665	37.785	1.00 17.16	MTGL
ATOM	652	Õ	ASP	84		-0.525	38.061	1.00 16.64	MTGL
ATOM	653	N	THR	85	43.978	1.406	38.152	1.00 16.98	MTGL
MOTA	654	CA	THR	85	42.889	0.837	38.943	1.00 17.09	MTGL
ATOM	655	CB	THR	85	43.169	1.056	40.456	1.00 17.53	MTGL
ATOM	656	OG1		85	42.211	0.337	41.239	1.00 20.04	MTGL
MOTA	657	CG2	THR	85	43.107	2.549	40.805	1.00 16.84	MTGL
ATOM	658	C	THR	85	41.543	1.460	38.546	1.00 16.53	MTGL
ATOM	659	ŏ	THR	85	41.481	2.245	37.598	1.00 16.58	MTGL
MOTA	660	N	TRP	186	40.477	1.100	39.264	1.00 15.91	MTGL
ATOM	661	CA	TRP	86	39.130	1.597	38.982	1.00 16.71	MTGL
ATOM	662	CB	TRP	86	38.166	1.291	40.143	1.00 15.33	MTGL
MOTA	663	CG	TRP	86	38.079	-0.151	40.525	1.00 17.03	MTGL
ATOM	664		TRP	86	37.311	-1.165	39.871	1.00 16.85	MTGL
ATOM	665	CE2	TRP	86	37.548	-2.378	40.560	1.00 17.49	MTGL
MOTA	666		TRP	86	36.448	-1.170	38.767	1.00 16.06	MTGL
ATOM	667	CD1	TRP	86	38.731	-0.768	41.555	1.00 16.85	MTGL MTGL
ATOM	668		TRP	86	38.417	-2.104	41.583	1.00 17.28	MTGL
MOTA	669	CZ2	TRP	86	36.951	-3.588	40.180	1.00 16.23	MTGL
ATOM	670	CZ3		86	35.853	-2.373	38.388	1.00 17.14 1.00 17.46	MTGL
MOTA	671	CH2	TRP	86	36.110	-3.566	39.095	1.00 17.40	MTGL
ATOM .	672	С	TRP	86	39.044	3.093	38.703	1.00 16.71	MTGL
ATOM	673	0	TRP	86	39.500	3.911	39.500 37.574	1.00 16.21	MTGL
MOTA	674	N	ALA	87	38.440	3.443	37.223	1.00 17.57	MTGL
MOTA	675	CA	ALA	87	38.249	4.845 5.124	35.809	1.00 16.32	MTGL
ATOM	676	CB	ALA	87	38.760	5.119	37.297	1.00 18.11	MTGL
ATOM	677	C	ALA	87	36.753	4.409	36.677	1.00 18.07	MTGL
MOTA	678	0	ALA	87	35,965 36.368	6.125	38.077	1.00 18.47	MTGL
MOTA	679	N	ASP	88 88	34.965	6.512		1.00 18.85	MTGL
ATOM	680	CA	ASP	88	34.287	5.730		1.00 18.63	MTGL
ATOM	681	CB	ASP	88	35.047	5.816		1.00 19.12	MTGL
ATOM	682	CC	ASP	88	35.352	6.940		1.00 18.34	MTGL
MOTA	683		ASP ASP	88	35.332	4.749		1.00 19.72	\mathtt{MTGL}
ATOM	684	C	ASP	88	34.932	8.021	_	1.00 18.13	MTGL
ATOM	685			88	35.980	8.656			MTGL
MOTA	68 6 68 7		ASP PRO	89	33.737	8.616		1.00 18.93	MTGL
ATOM	688		PRO	89	32.382	8.046		1.00 19.94	MTGL
MOTA	689		PRO	89	33.672	10.066		1.00 19.49	MTGL
ATOM ATOM	690		PRO	89	32.174	10.327		1.00 19.80	MTGL
ATOM	691		PRO		31.555	9.263		1.00 19.69	MTGL
ATOM	692		PRO		34.476	10.600		1.00 19.90	MTGL
ATOM	693		PRO		34.833	11.778		1.00 20.62	MTGL
ATOM	694		ALA		34.760	9.743		1.00 18.70	MTGL
MOTA	695				35.519	10.164		1.00 19.35	MTGL

Fig. 1 cont.

		A D	7 T	90	34.818	9.685	43.457	1.00 17.48	MTGL
ATOM	696		ALA ALA	90	36.964	9.674	42.162	1.00 18.63	MTGL
MOTA	697		ALA	90	37.730	9.988	43.071	1.00 19.58	MTGL
ATOM	698		HIS	91	37.333	8.901	41.145	1.00 17.84	MTGL
ATOM	699		HIS	91	38.698	8.391	41.039	1.00 17.68	MTGL
ATOM	700	CA		91	38.833	7.000	41.679	1.00 18.34	MTGL
ATOM	701	CB CG	HIS HIS	91	38,298	6.910	43.072	1.00 20.31	MTGL
MOTA	702	CD2		91	38.927	6.936	44.272	1.00 19.87	MTGL
ATOM	703	ND1		91	36.953	6.784	43.344	1.00 18.50	MTGL
ATOM	704 705	CE1		91	36.775	6.736	44.653	1.00 20.43	MTGL
MOTA		NE2		91	37,956	6.826	45.238	1.00 21.64	MTGL
ATOM	706		HIS	91	39.177	8.280	39.597	1.00 16.55	MTGL
MOTA	707	C	HIS	91	38,661	7,478	38.823	1.00 16.39	MTGL
ATOM	708	О И	GLN	92	40.169	9.087	39.246	1.00 15.52	MTGL
ATOM	709		GLN	92	40.760	9.064	37.911	1.00 15.68	MTGL
ATOM	710	CA	GLN	92	40.281	10.255	37.072	1.00 14.49	MTGL
MOTA	711	CB CG	GLN	92	38.786	10.229	36.702	1.00 13.93	MTGL
ATOM	712	CD	GLN	92	38.413	9.127	35.699	1.00 14.84	t MTGL
MOTA	713 714		GLN	92	39.173	8.614	34.779	1.00 15.41	MTGL
ATOM	715		GLN	92	37.221	8.559	35.861	1.00 14.23	MTGL
MOTA	716	C	GLN	92	42.254	9,166	38.190	1.00 15.81	MTGL
MOTA	717	Ö	GLN	92	42.925	10.108	37.782	1.00 16.26	MTGL
MOTA MOTA	718	И	THR	93	42.759	8.169	38.902	1.00 16.47	MTGL
ATOM	719	CA	THR	93	44.156	8.136	39.302	1.00 17.33	MTGL
ATOM	720	CB	THR	93	44.387	7.062	40.364	1.00 17.41	MTGL
MOTA	721		THR	93	43,433	7,239	41.417	1.00 19.90	MTGL
ATOM	722	CG2		93	45.800	7.177	40.944	1.00 19.68	MTGL
ATOM	723	C	THR	93	45.136	7.925	38.165	1.00 17.55	MTGL
MOTA	724	ŏ	THR	93	45.035	6.973	37.390	1.00 17.01	MTGL
ATOM	725	Ň	MET	94	46.093	8.839	38.089	1.00 17.63	MTGL
ATOM	726	CA	MET	94	47.131	8.820	37.079	1.00 18.68	MTGL
ATOM	727	CB	MET	94	48.144	9.926	37.383	1.00 21.10	MTGL
ATOM	728	CG	MET	94	49.195	10.133	36.315	1.00 23.55	MTGL
ATOM	729	SD	MET	94	48.474	10.956	34.894	1.00 27.41	MTGL MTGL
ATOM	730	CE	MET	94	48.342	12.657	35.533	1.00 25.13	MTGL
ATOM	731	С	MET	94	47.854	7.476	37.064	1.00 18.43	MTGL
ATOM	732	0	MET	94	48.179	6.925	38.113	1.00 18.13	MTGL
ATOM	733	N	PRO	95	48.088	6.914	35.871	1.00 17.41	MTGL
. ATOM	734	CD	PRO	95	47.534	7.255	34.551	1.00 16.67	MIGL
MOTA	735	CA	PRO	95	48.797	5.631	35.834	1.00 17.83 1.00 17.25	MTGL
MOTA	736	CB	PRO	95	48.814	5.287	34.347	1.00 17.23	MTGL
ATOM	737	CG	PRO	95	47.544	5.914	33.843 36.371	1.00 17.33	MTGL
ATOM	738	С	PRO	95	50.202	5.903		1.00 17.30	MTGL
ATOM	739	0	PRO	95	50.784	6.952			MTGL
MOTA	740		ALA	96	50.746	4.978			MTGL
MOTA	741	CA	ALA	96	52.082	5.177		1.00 19.66	MTGL
ATOM	742		ALA	96	52.470	3.983			MTGL
MOTA	743	С	ALA	96	53.095	5.357			MTGL
ATOM	744		ALA	96	53.081	4.617			MTGL
MOTA	745		GLY	97 27	53.959	6.356			MTGL
MOTA	746			97	54.967	6.595 7.644		^^	MTGL
MOTA	747		GLY	97	54.611	8.144			MTGL
ATOM	748		GLY	97	55.491	7.982			MTGL
ATOM	749		TRP	98	53.332	8.978			MTGL
ATOM	750			98	52.902	8.795			MTGL
MOTA	751			98	51.415 51.106				MTGL
ATOM	752			98	49.987				MTGL
ATOM	753	CD	2 TRP	98	49.96/	1.391	J.J.J.		

Fig. 1 cont.

				0.0	50.082	6.093	31.006	1.00 16.95	MTGL
ATOM		CE2		98	48.914	8.213		1.00 15.48	MTGL
ATOM	755		TRP	98 98	51.810	6.406	32.385	1.00 18.21	MTGL
ATOM	756			-	51.202	5.511	31.538	1.00 17.45	MTGL
MOTA	757	NE1		98	49.140	5.580	30.103	1.00 17.12	MTGL
ATOM	758		TRP	98	47.974	7.704	30.257	1.00 15.71	MTGL
MOTA	759	CZ3	TRP	98	48.098	6.399	29.740	1.00 16.54	MTGL
MOTA	760		TRP	98	53.156	10.401	34.056	1.00 20.28	MTGL
ATOM	761	C	TRP	98	52.958	10.706	35.230	1.00 19.92	MTGL
MOTA	762	0	TRP	98	53.593	11.295	33.156	1.00 21.71	MTGL
ATOM	763	N	PRO	99		11.048	31.725	1.00 22.15	MTGL
MOTA	764	CD	PRO	99	53.852 53.875	12.693	33.505	1.00 22.69	MTGL
MOTA	765	CA	PRO	99		13.205	32.269	1.00 22.58	MTGL
MOTA	766	CB	PRO	99	54.610 53.938	12.454	31.163	1.00 22.80	MTGL
ATOM	767	CG	PRO	99	52.598	13.483	33.797	1.00 23.10	MTGL
ATOM	768	С	PRO	99		13.156	33.277	1.00 23.44	MTGL
MOTA	769	0	PRO	99 .	51.530	14.522	34.621	1.00 22.96	MTGL
ATOM	770	N	SER	100	52.716		34.921	1.00 23.06	MTGL
MOTA	771	CA	SER	100	51.572	15.353	36.445	1.00 24.32	MTGL
ATOM	772	CB	SER	100	51.714	15.831	37.353	1.00 26.38	MTGL
MOTA	773	OG	SER	100	51.658	14.746	34.115	1.00 22.44	MTGL
ATOM	774	С	SER	100	51.332	16.574	34.032	1.00 22.25	MTGL
ATOM	775	0	SER	100	50.202	17.051	33.480	1.00 22.23	MTGL
ATOM	776	N	ASP	101	52.379	17.098	32.639	1.00 23.28	MTGL
MOTA	דדד	CA	ASP	101	52.208	18.283	32.254	1.00 24.51	MTGL
ATOM	778	CB	ASP	101	53.565	18.890	31.352	1.00 25.84	MTGL
MOTA	779	CG	ASP	101	54.382	17.986	31.842	1.00 26.46	MTGL
MOTA	780	OD1		101	54.886	16.954	30.152	1.00 25.84	MTGL
MOTA	781	QD2		101	54.515	18.310	31.386	1.00 22.28	MTGL
MOTA	782	С	ASP	101	51.411	17.933	30.743	1.00 21.59	MTGL
ATOM	783	0	ASP	101	51.667	16.915		1.00 21.77	MTGL
ATOM	784	N	ILE	102	50.452	18.787	31.042 29.890	1.00 21.42	MTGL
ATOM	785	CA	ILE	102	49.584	18.548	29.663	1.00 20.48	MTGL
MOTA	786	CB	IĻE	102	48.623	19.738	29.313	1.00 20.99	MTGL
ATOM	787		LLE	102	49.411	20.998	28.560	1.00 21.44	MTGL
ATOM	788	CG1		102	47.617	19.392	28.879	1.00 19.62	MTGL
MOŢA	789	CD1	ILE	102	46.730	18.200	28.573	1.00 21.71	MTGL
MOTA	790	С	ILE	102	50.281	18.196	27.896	1.00 20.84	MTGL
MOTA	791	0	ILE	102	49.861	17.258	28.201	1.00 21.01	MTGL
MOTA	792	32	ASP.	103	51.336	18.918	26.945	1.00 22.44	MTGL
MOTA	793	CA	ASP	103	52.012	18.608 19.523	26.716	1.00 24.91	MTGL
MOTA	794	, CB	ASP	103	53.219		26.370	1.00 27.06	MTGL
MOTA	795	CG	ASP	103	52.821	20.942	26.070	1.00 27.99	MTGL
MOTA	796		LASP	103	51.633	21.178 21.823	26.385	1.00 28.69	MTGL
ATOM	797	OD:		103	53.703	17.160	26.886	1.00 22.61	MTGL
MOTA	798	С	ASP	103	52.478		25.948	1.00 23.39	MTGL
ATOM	799	0	ASP	103	52.144	16.435	27.885	1.00 21.79	MTGL
ATOM	800	Ŋ	ASN	104	53.244	16.734		1.00 22.22	MTGL
ATOM	801	CA	ASN	104	53.751	15.366		1.00 23.92	MTGL
ATOM	802	CB	ASN	104	54.912	15.244	28.884		MTGL
MOTA	803			104	56.149	15.977			MTGL
ATOM	804		1 ASN	104	56.715				MTGL
ATOM	805		2 ASN	104	56.570	16.989			MTGL
ATOM	806		ASN	104	52.699		28.191		MTGL
MOTA	807	0	ASN	104	52.774				MTGL
ATOM	808		LEU	105	51.722				MTGL
MOTA	809			105	50.663		29.361		MTGL
ATOM	810			105	49.743				MTGL
ATOM	811	CG	LEU	105	48.568	13.339	30.842	1.00 18.64	1,1727
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Fig. 1 cont.

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ATOM	812	CD1	LEU	105	49.089	12.019	31.413	1.00	15.72	MTGL
ATOM	813	CD2		105	47.690	14.040	31.860	1.00	17 06	MTGL
ATOM	814	С	LEU	105	49.841	13.392	28.109	1.00	20.55	MTGL
ATOM	815	0	LEU	105	49.506	12.237	27.839	1.00	20.48	MTGL
					49.521		27.346		20.24	
MOTA	816	N	SER	106		14.435				MTGL
MOTA	817	CA	SER	106	48.746	14.264	26.124	1.00	21.47	MTGL
ATOM	818	CB	SER	106	48.514	15.610	25.437	1 00	22.23	MTGL
ATOM	819	OG	SER	106	47.695	16.447	26.235	1.00	27.30	MTGL
MOTA	820	С	SER	106	49.484	13.338	25.173	1.00	20.88	MTGL
ATOM	821	ō	SER	106	48.884	12.487	24.527		19.42	MTGL
MOTA	822	N	TRP	107	50.795	13.513	25.096	1.00	22.85	MTGL
ATOM	823	CA	TRP	107	51.623	12.696	24.223	1 00	24.06	MTGL
ATOM	824	CB	TRP	107	53.033	13.282	24.164		27.94	MTGL
ATOM	825	CG	TRP	107	53.780	12.934	22.924	1.00	32.46	MTGL
ATOM	826	CD2	TRP	107 ·	55.136	13:276	22.621	1 00	35.03	MTGL
		-								
ATOM	827	CE2	TRP	107	55.414	12. 7 76	21.328	1.00	36.06	MTGL
ATOM	828	CE3	TRP	107	56.141	13.971	23.309	1.00	36.31	MTGL
MOTA	829	CD1	TRD	107	53.303	12.249	21.839	1 00	33.32	MTGL
ATOM	830	NE1	TRP	107	54.280	12.148	20.877	1.00	35.87	MTGL
ATOM	831	CZ2	TRP	107	56.662	12.934	20.715	1.00	36.87	MTGL
ATOM	832	CZ3		107	57.381	14.130	22.698		37.64	MTGL
ATOM	833	CH2	TRP	107	57.627	13.617	21.410		37.50°	MTGL
MOTA	834	С	TRP	107	51.674	11.250	24.725	1.00	23.66	MTGL
MOTA	835	0	TRP	107	51.632	10.306	23.929		22.42	MTGL
ATOM	836	N	LYS	108	51.754	11.085	26.045	1.00	21.87	MTGL
MOTA	837	CA	LYS	108	51.810	9.758	26.654	1.00	21.77	MTGL
ATOM	838		LYS	108	52.012	9.870	28.167		22.68	MTGL
		CB								
ATOM	839	CG	LYS	108	52.928	8.818	28.787	1.00	25,44	MTGL
ATOM	840	CD	LYS	108	52.756	7.420	28.208	1.00	25.37	MTGL
ATOM	841	CE		108		6.436				MTGL
			LYS		53.657		28.948		26.82	
ATOM	842	NZ	LYS	108	53.912	5.168	28.202	1.00	25.16	MTGL
MOTA	843	С	LYS	108	50.502	9.016	26.400	1.00	21.11	MTGL
ATOM	844	0	LYS	108	50.499	7.825	26.082		20.02	MTGL
MOTA	845	N	LEU	109	49.394	9.733	26.569	1.00	20.01	MTGL
ATOM	846	CA	LEU	109	48.069	9.165	26.378	1.00	19.28	MTGL
ATOM	847	СВ	LEU	109	46.998	10.210	26.701		17.83	MTGL
ATOM	848	CG	LEU	109	45.541	9.782	26.544		18.16	
ATOM	849	CD1	LEU	109	45.278	8.500	27.331	1.00	16.64	\mathtt{MTGL}
MOTA	850	CDS	LEU	109	44.639	10.912	27.023	7 00	17.12	MTGL
MOTA	851	С	LEU	109	47.922	8.689	24.941		19.15	MTGL
MOTA	852	0	LEU	109	47.356	7.630	24.681	1.00	17.95	MTGL
ATOM	853	N	TYR	110	48.439	9.485	24.013	1.00	19.31	MTGL
MOTA	854	CA	TYR	110	48.390	9.141	22.602		20.23	MTGL
ATOM	855	CB	TYR	110	48.928	10.308	21.765	1.00	20.77	MTGL
ATOM	856	CG	TYR	110	49.112	9.988	20.301	1.00	22.28	MTGL
										MTGL
ATOM	857		TYR	110	50.324	9.483	19.827		22.42	
ATOM	858	CE1	TYR	110	50.500	9.174	18.478	1.00	23.01	MTGL
ATOM	859	CD2	TYR	110	48.072	10.179	19.388	1.00	21.90	MTGL
										MTGL
ATOM	860		TYR	110		9.873	18.033		22,98	
ATOM	861	CZ	TYR	110	49.453	9.373	17.589	1.00	22.70	MTGL
ATOM	862	OH	TYR	110	49.628	9.075	16.261	1.00	22.60	MTGL
						7.873				
ATOM	863	Č	TYR	110	49.209		22.351		20.36	MTGL
ATOM	864	0	TYR	110	48.713	6.915	21.753	1.00	19.75	MTGL
MOTA	865	N	NZA	111	50.453	7.864	22.826		19.95	MTGL
ATOM	866	CA	ASN	111	51.333	6.712	22.650		20.79	MTGL
MOTA	867	СВ	ASN	111	52.691	6.944	23.316	1.00	22.26	MTGL
ATOM	868	CG	ASN	111	53.496	8.030	22.642		26.38	MTGL
MOTA	869	OD1								MTGL
WION	005	ODT	なつに	111	53.175	8.463	21.534	7.00	25.33	LIGI.

Fig. 1 cont.

MOTA	870	ND2	NZA	111	54.556	8.463	23.317	1.00 29.11	MTGL
ATOM	871		ASN	111	50.736	5.445	23.234	1.00 20.44	MTGL
				111	50.764	4.391	22.605	1.00 20.22	MTGL
ATOM	872	0	ASN			5.551	24.452	1.00 19.27	MTGL
ATOM	873		TYR	112	50.218				MTGL
ATOM	874	ÇA	TYR	112	49.622	4.406	25.123	1.00 18.94	
ATOM	875	CB	TYR	112	49.131	4.801	26.517	1.00 16.74	MTGL
ATOM	876	CG	TYR	112	48.211	3.770	27.137	1.00 17.22	MTGL
ATOM	877	CD1		112	48.723	2.632	27.766	1.00 15.42	MTGL
	878	CE1		112	47.876	1.671	28.311	1.00 17.32	MTGL
MOTA					46.827	3.916	27.065	1.00 15.87	MTGL
ATOM	879	CD2		112			27.604	1.00 17.72	MTGL
ATOM	880	CE2		112	45.971	2.960			
MOTA	881	CZ	TYR	112	46.500	1.844	28.225	1.00 16.39	MTGL
ATOM	882	OH	TYR	112	45.653	0.907	28.766	1.00 18.06	MTGL
ATOM	883	С	TYR	112	48.449	3.832	24.330	1.00 18.50	MTGL
ATOM	884	ō	TYR	112	48.358	2.622	24.129	1.00 17.86	MTGL
ATOM	885	N	THR	113	47.545	4.709	23.903	1.00 18.56	MTGL
				113	46.372	4.288	23.152	1.00 18.24	MTGL
MOTA	886	CA	THR			5.474	22,930	1.00 17.98	MTGL
MOTA	887	CB	THR	113	45.408			1.00 16.20	MTGL
ATOM	888	OG1		113	45.017	6.014	24.198		
MOTA	889	CG2	THR	113	44.158	5.021	22.184	1.00 17.01	MTGL
ATOM	890	С	THR	113	46.765	3.682	21.805	1.00 18.67	MTGL
ATOM	891	0	THR	113	46.272	2.619	21.423	1.00 18.43	MTGL
ATOM	892	N	LEU	114	47.655	4.360	21.090	1.00 19.14	MTGL
ATOM	893	CA	LEU	114	48.114	3.873	19.797	1.00 20.50	MTGL
				114	49.133	4.848	19.197	1.00 20.12	MTGL
MOTA	894	CB	LEU				17.929	1.00 21.74	MTGL
ATOM	895	CG	LEU	114	49.864	4.396			MTGL
MOTA	896		LEU	114	48.866	4.214	16.794	1.00 21.80	
ATOM	897	CD2	ren	114	50.924	5.430	17.547	1.00 22.25	MTGL
ATOM	898	С	LEU	114	48.753	2.498	19.984	1.00 20.96	MTGL
MOTA	899	0	LEU	114	48.441	1.551	19.263	1.00 21.53	MTGL
ATOM	900	N	ASP	115	49.650	2.399	20.961	1.00 21.00	MTGL
ATOM	901	CA	ASP	115	50.335	1.148	21.252	1.00 21.18	MTGL
	902	CB	ASP	115	51.276	1.331	22.442	1.00 22.68	MTGL
MOTA					51.957	0.041	22.843	1.00 24.76	MTGL
ATOM	903	CG	ASP	115				1.00 26.71	MTGL
MOTA	904		ASP	115	52.826	-0.429	22.078		MTGL
MOTA	905	OD2	ASP	115	51.616	-0.509	23.917	1.00 25.94	
ATOM	906	C	ASP	115	49.351	0.018	21,561	1.00 21.01	MTGL
MOTA	907	0	ASP	115	49.461	-1.078	21.012	1.00 20.38	MTGL
ATOM	908	N	ALA	116	48.404	0.287	22.456	1.00 19.72	MTGL
ATOM	909	CA	ALA	116	47.410	-0.711	22.833	1.00 19.79	MTGL
MOTA	910	CB	ALA	116	46.501	-0.163	23.923	1.00 19.04	MTGL
	911		ALA	116	46.578	-1.140	21.627	1.00 18.78	MTGL
ATOM		C				-2.323	21.448	1.00 18.71	MTGL
ATOM	912	0	ALA	116	46.302			1.00 18.51	MTGL
ATOM	913	N	ALA	117	46.184	-0.172	20.806		MTGL
ATOM	914	CA	ALA	117	45.384	-0.456	19.616	1.00 19.07	
MOTA	915	CB	ALA	117	45.012	0.840	18.913	1.00 17.76	MTGL
ATOM	916	Ç	ALA	117	46.144	-1.372	18.662	1.00 19.00	MTGL
ATOM	917	ò	ALA	117	45.588	-2.344	18.157	1.00 20.94	MTGL
MOTA	918	N	ASN	118	47.414	-1.064	18.421	1.00 19.11	MTGL
				118	48.234	-1.880	17.530	1.00 20.09	MTGL
ATOM	919	ÇA	ASN		49.594	-1.214	17.280	1.00 19.53	MTGL
ATOM	920	ĊВ	ASN	118				1.00 21.06	MTGL
MOTA	921	CG	ASN	118	49.481	0.043	16.432		
MOTA	922		ASN	118	48.591	0.158	15.584	1.00 22.85	MTGL
MOTA	923	ND2	ASN	118	50.394	0.984	16.644	1.00 19.62	MTGL
ATOM	924	C	ASN	118	48.446	-3.294	18.069	1.00 20.53	MTGL
ATOM	925	ō	ASN	118	48.509	-4.250	17.298	1.00 20.72	MTGL
MOTA	926	Й	LYS	119	48.570	-3.427	19.389	1.00 20.26	MTGL
	927		LYS	119	48.755	-4.745	19.992	1.00 19.69	MTGL
ATOM	761	CA	пιэ	エエコ	70./70	3.173	4000	2.00 20.00	

Fig. 1 cont.

				110	40 134	-4.616	21.468	1,00 20.25	MTGL
MOTA	928	CB	LYS	119	49.134				
ATOM	929	CG	LYS	119	50.589	~4.225	21.668	1.00 23.15	MTGL
ATOM	930	CD	LYS	119	50.933	-4.015	23.131	1.00 25.43	MTGL
ATOM	931	CE	LYS	119	52.378	-3.533	23.273	1.00 26.95	\mathtt{MTGL}
MOTA	932	NZ	LYS	119	52,701	-3.126	24.666	1.00 26.48	MTGL
				119	47.482	-5.570	19.843	1.00 18.61	MTGL
MOTA	933	C	LYS		•			1.00 16.84	MTGL
ATOM	934	0	LYS	119	47.533	-6.777	19.615		
MOTA	935	N	LEU	120	46.339	-4.911	19.975	1.00 17.54	MTGL
MOTA	936	CA	LEU	120	45.064	-5.599	19.820	1.00 18.74	MTGL
ATOM .	937	ÇB	LEU	120	43.909	-4.643	20.144	1.00 17.57	MTGL
ATOM .	938	CG	LEU	120	43.736	-4.330	21.635	1.00 17.26	MTGL
ATOM	939	CD1		120	42.836	-3.117	21.830	1.00 17.85	MTGL
ATOM	940	CD2		120	43.152	-5.549	22.325	1.00 16.86	MTGL
ATOM	941	C	LEU	120	44.976	-6.086	18.372	1.00 18.39	MTGL
						· -7.243	18.116	1.00 19.13	MTGL
MOTA	942	0	LEU	120					MTGL
ATOM	943	N	GLN	121	45.273	-5.193	17.434	1.00 19.05	
ATOM	944	CA	GLN	121	45.245	-5.524	16.013	1.00 20.51	MTGL
MOTA	945	CB	GLN	121	45.715	-4.324	15.182	1.00 20.27	MTGL
ATOM	946	CG	GLN	121	45.927	-4.606	13.694	1.00 19.88	MTGL
ATOM	947	CD	GLN	121	44.677	-5.116	12.998	1.00 20.20	\mathtt{MTGL}
MOTA	948	OE1		121	43.565	-4.680	13.291	1.00 19.32	MTGL
ATOM	949		GLN	121	44.859	-6.035	12.055	1.00 20.98	MTGL
	950		GLN	121	46.142	-6.723	15.734	1.00 20.78	MTGL
ATOM		C						1.00 21.20	MTGL
MOTA	951	0	GLN	121 .	45.729	-7.672	15.078		MTGL
ATOM	952	N	ASN	122	47.369	-6.676	16.242	1.00 20.58	
ATOM	953	CA	ASN	122	48.322	-7.762	16.037	1.00 22.39	MTGL
ATOM	954	CB	ASN	122	49.685	-7.371	16.611	1:00 24.20	MTGL
MOTA	955	CG	ASN	122	50.350	-6.260	15.817	1.00 26.36	MTGL
ATOM	956	OD1	ASN	122	51.298	-5.630	16.285	1.00 29.40	MTGL
ATOM	957		ASN	122	49.863	-6.021	14.605	1.00 26.25	MTGL
ATOM	958	C	ASN	122	47.859	-9.082	16.646	1.00 22.40	MTGL
ATOM	959	ŏ	ASN	122		-10.153	16.243	1.00 23.25	MTGL
							17.616	1.00 21.34	MTGL
MOTA	960	N	ALA	123	46.957	-9.005			MTGL
ATOM	961	CA	ALA	123		-10.209	18.252	1.00 21.19	
ATOM	962	CB	ALA	123	46.151	-9.939	19.730	1.00 21.28	MTGL
MOTA	963	С	ALA	123		-10.669	17.545	1.00 20.31	MTGL
MOTA	964	0	ALA	123	44.512	-11.621	17.981	1.00 21.19	MTGL
ATOM	965	N	GLY	124	44.813	~9.985	16.457	1.00 20.00	MTGL
MOTA	966	CA	GLY	124	43.621	-10.332	15.705	1.00 19.34	MTGL
ATOM	967	С	GLY	124	42.338	-9.853	16.367	1.00 20.32	MTGL
ATOM	968	ŏ	GLY	124		-10.376	16.098	1.00 19.71	MTGL
ATOM	969	N	ILE	125	42.450	-8.855	17.239	1.00 18.85	MTGL
	970	CA	ILE	125	41.281		17.928	1.00 17.97	MTGL
ATOM						-8.279	19.465	1.00 18.21	MTGL
ATOM	971	CB	ILE	125	41.502				
MOTA	972	CG2		125	40.264	-7.709	20.149	1.00 18.39	MTGL
ATOM	973	CG1			41.807	-9.681	20.013	1.00 16.78	MTGL
ATOM	974	CD1	ILE	125	40.682	-10.694	19.808	1.00 15.33	MTGL
ATOM	975	C	ILE	125	40.936	-6.908	17.460	1.00 18.72	MTGL
ATOM	976	0	ILE	125	41,682	~5.959	17.718	1.00 18.82	MTGL
ATOM	977	N	GLN	126	39.810	-6.771	16.769	1.00 17.38	MTGL
ATOM	978	CA	GLN	126	39.355	-5.463	16.310	1.00 17.54	MTGL
	979	CB	GLN	126	39.059	~5.459	14.810	1.00 17.95	MTGL
MOTA								1.00 17.33	MTGL
ATOM	980	CG	GLN	126	40.267	-5.634	13.905		
ATOM	981	CD	GLŊ	126	40.704	-7.082	13.784	1.00 19.41	MTGL
ATOM	982		GLN	126	39.874	-7.991	13.722	1.00 18.45	MTGL
ATOM	983	NE2	GLN	126	42.014	-7.302	13.731	1.00 18.37	MTGL
ATOM	984	C	GLN	126	. 38.078	-5.152	17.073	1.00 17.01	MTGL
ATOM	985	0	GLN	126	36.990	-5.578	16.686	1.00 17.42	MTGL
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Fig. 1 cont.

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ATOM	986	N	PRO	127	38.196	-4.424	18.189	1.00 17.14	MTGL
MOTA	987	CD	PRO	127	39.397	-3.833	18.803	1.00 16.94	MTGL
MOTA	988	CA	PRO	127	36.990	-4.103	18.954	1.00 17.76	MTGL
ATOM	989	CB	PRO	127	37.534	-3.333	20.162	1.00 17.60	MTGL
MOTA	990	CG	PRO	127	38.806	-2.730	19.644	1.00 20.07	MTGL
ATOM	991	Ċ	PRO	127	36.004	-3.290	18.130	1.00 17.06	mtgl Mtgl
MOTA	992	0	PRO	127	36.400	-2.472	17.303	1.00 18.03 1.00 17.80	MTGL
ATOM	993	N	THR	128	34.719	-3.536	18.340	1.00 17.50	MTGL
MOTA	994	CA	THR	128	33.688	~2.803	17.620	1.00 17.39	MTGL
ATOM	995	CB	THR	128	32.357	-3.582	17.615	1.00 17.44	MTGL
ATOM	996		THR	128	32.035	-3.994 -4.816	18.951 16.717	1.00 17.44	MTGL
MOTA	997	CG2		128 .	32.467	-1.451	18.310	1.00 17.94	MTGL
MOTA	998	Ç	THR	128	33.499 33.086	-0.476	17.683	1.00 16.71	MTGL
ATOM	999	0	THR	128	33.834	-1.397	19.600	1.00 16.54	MTGL
MOTA	1000	N CA	ILE	129 129	33.701	-0.161	20.373	1.00 16.74	MTGL
MOTA	1001 1002	CB	ILE	129	32.426	-0.166	21.249	1.00 17.47	MTGL
ATOM	1002	CG2		129	32.323	1.138	22.032	1.00 16.90	MTGL
MOTA MOTA	1003	CG1		129	31.182	-0.340	20.380	1.00 18.59	MTGL
MOTA	1005	CDI		129	29.913	-0.501	21.189	1.00 18.26	MTGL
ATOM	1005	C	ILE	129	34.878	0.056	21.317	1.00 16.72	MTGL
ATOM	1007	ŏ	ILE	129	35.361	-0.883	21.949	1.00 16.12	MTGL
MOTA	1008	N	VAL	130	35.329	1.303	21.410	1.00 16.38	MTGL
ATOM	1009	CA	VAL	130	36.413	1.666	22.313	1.00 16.43	MTGL
ATOM	1010	СВ	VAL	130	37.738	1.891	21.568	1.00 16.85	MTGL
MOTA	1011	CG1	VAL	130	38.783	2.444	22.532	1.00 15.96	MTGL
ATOM	1012	CG2	VAL	130	38.224	0.581	20.958	1.00 16.65	MTGL
ATOM	1013	С	VAL	130	36.040	2.965	23.020	1.00 16.57	MTGL
MOTA	1014	0	VAL	130	35.807	3.981	22.369	1.00 17.33	MTGL
MOTA	1015	N	SER	131	35.955	2.931	24.347	1.00 15.26	MTGL
ATOM	1016	CA	SER	131	35.640	4.142	25.08B	1.00 14.32	MTGL
MOTA	1017	CB	SER	131	34.741	3.840	26.296	1.00 13.74	MTGL
MOTA	1018	OG	SER	131	35.427	3.100	27.299	1.00 14.55	MTGL
MOTA	1019	С	SER	131	36.957	4.737	25.563	1.00 13.67	MTGL
ATOM	1020	0	SER	131	37.812	4.024	26.094	1.00 14.63	MTGL MTGL
MOTA	1021	N	ILE	132	37.140	6.033	25.349	1.00 12.98	MTGL
MOTA	1022	CA	ILE	132	38.362	6.684	25.791	1.00 13.07	MTGL
MOTA	1023	CB	ILE	132	38.793	7.796	24.811	1.00 13.05 1.00 14.24	MTGL
ATOM	1024		ILE	132	39.419	7.169	23.573 24.397	1.00 13.32	MTGL
MOTA	1025		ILE	132	37.591	8.649	23.429	1.00 13.32	MTGL
MOTA	1026		ILE	132 132	37.960 38.103	9.760 7.234	27.188	1.00 13.33	MTGL
ATOM	1027	C	ILE	132	37.800	8.415	27.372	1.00 12.93	MTGL
MOTA MOTA	1028 1029	O N	GLY	133	38.206	6.339	28.170	1.00 12.78	MTGL
ATOM	1029	CA	GLY	133	37.957	6.703	29.552	1.00 13.26	MTGL
ATOM	1030	Ç	GLY	133	36.687	6.040	30.066	1.00 14.41	MTGL
ATOM	1032	ŏ	GLY	133	35.821	5.638	29.279	1.00 14.45	MTGL
MOTA	1033	N	ASN	134	36.573	5.915	31.385	1.00 14.34	MTGL
ATOM	1034	CA	ASN	134	35.393	5.311	31.995	1.00 14.81	MTGL
ATOM	1035	CB	ASN	134	35.797	4.063	32.780	1.00 14.03	MTGL
MOTA	1036	ÇĞ	ASN	134	34.602	3.307	33.321	1.00 15.54	MTGL
ATOM	1037		ASN	134	33.932	2.558	32.596	1.00 14.69	MTGL
ATOM	1038		ASN	134	34.311	3.515	34.599	1.00 13.31	MTGL
ATOM	1039	Ç	ASN	134	34.727	6.328	32.929	1.00 15.45	MTGL
ATOM	1040	ò	ASN	134	35.355	6.823	33.865	1.00 14.99	MTGL
ATOM	1041	N	GLU	135	33.458	6.632	32.672	1.00 15.32	MTGL
MOTA	1042	CA	GĻŪ	135	32.708	7.600	33.480	1.00 16.19	MTGL
MOTA	1043	CB	GLU	135	32.225	6.948	34.780	1.00 16.84	MTGL

Fig. 1 cont.

ATOM	1044	CG	GLU	135	31.360	5.710	34.571	1.00 18.65	MTGL
ATOM	1045	CD	GLU	135	30.758	5.173	35.862	1.00 19.18	MTGL
	1046								
ATOM		OE1		135	31.449	5.200	36.905	1.00 20.99	MTGL
ATOM	1047	OE2	GLU	135	29.602	4.705	35.829	1.00 16.99	MTGL
MOTA	1048	С	GLU	135	33.553	8.834	33.806	1.00 16.49	MTGL
ATOM	1049	0	GLU	135	33.777	9.153	34.974	1.00 15.93	MTGL
ATOM	1050	N	ILE	136	34.004	9.536	32.770	1.00 15.57	MTGL
ATOM	1051	CA	ILE	136	34.846	10.712	32.957	1.00 16.13	MTGL
MOTA	1052	CB	ILE	136	35.802	10.887	31.756	1.00 16.05	MTGL
ATOM	1053	CG2	ILE	136	36.783	9.719	31.706	1.00 16.66	MTGL
ATOM	1054	CG1	ILE	136	35.001	10.956	30.451	1.00 16.40	MTGL
ATOM	1055		ILE	136	35.858	11.171	29.211	1.00 14.50	MTGL
ATOM	1056	C	ILE	136					
					34.060	12.006	33.168	1.00 16.79	MTGL
ATOM	1057	0	ILE	136	34.457	13.067	32.697	1.00 16.67	MTGL
ATOM	1058	N	ARG	137	32.949	11.909	33.890	1.00 17.28	MTGL
ATOM	1059	CA	ARG	137	32.099	13.057	34.170	1.00 18.25	MTGL
ATOM	1060	CB	ARG	137	30.884	12.612	34.976	1,00 20.33	MTGL
ATOM	1061	CG	ARG	137	29.879	13.712	35.248		
ATOM	1062							1.00 22.61	MTGL
		CD	ARG	137	29.087	13.370	36.487	1.00 26.40	MTGL
ATOM	1063	NE	ARG	137	29.837	13.668	37.696	1.00 28.06	MTGL
ATOM	1064	CZ	ARG	137	29.643	13.076	38.869	1.00 28.40	MTGL
ATOM	1065	NH1	ARG	137	28.726	12.132	39.006	1.00 27.39	MTGL
ATOM	1066	NH2	ARG	137	30.355	13.459	39.918	1.00 30.54	· MTGL
MOTA	1067	С	ARG	137	32.849	14.145			
							34.937	1.00 19.12	MTGL
ATOM	1068	0	ARG	137	32.537	15.327	34.812	1.00 19.19	MTGL
MOTA	1069	N	ALA	138	33.832	13.744	35.738	1.00 17.89	MTGL
ATOM	1070	CA	ALA	138	34.626	14.708	36.487	1.00 18.61	MTGL
ATOM	1071	CB	ALA	138	34.679	14.320	37.965	1.00 18.89	MTGL
ATOM	1072	С	ALA	138	36.028	14.744	35.888	1.00 18.04	MTGL
ATOM	1073	ō	ALA	138	37.003	15.050	36.573	1.00 18.75	
									MTGL
MOTA	1074	N	GLY	139	36.119	14.415	34.603	1.00 17.60	MTGL
ATOM	1075	CA	GLY	139	37.401	14.424	33.920	1.00 16.74	MTGL
ATOM	1076	С	GLY	139	38.141	13.103	33.979	1.00 17.00	MTGL
ATOM	1077	0	GLY	139	37.558	12.061	34.303	1.00 15.56	MTGL
ATOM	1078	N	LEU	140	39.430	13.150	33.653	1.00 16.36	MTGL
MOTA	1079	CA	TEO	140	40.288	11.965	33.666	1.00 16.91	MTGL
ATOM	1080	CB	LEU	140	40.254				
						11.255	32.308	1.00 16.55	MTGL
ATOM	1081	CG	LEU	140	40.965	11.954	31.137	1.00 17.14	MTGL
ATOM	1082	CD1		140	41.157	10.962	29.985	1.00 17.61	MTGL
ATOM	1083	CD2	LEU	140	40.158	13.157	30.673	1.00 16.51	MTGL
ATOM	1084	C	LEU	140	41,731	12.366	33.961	1.00 16.82	MTGL
ATOM	1085	0	LEU	140	42.078	13.549	33.919	1.00 16.86	MTGL
MOTA	1086	N	LEU	141	42.566	11.373	34.254	1.00 16.21	
ATOM	1087	CA							MTGL
			LEU	141	43.979	11.616	34.521	1.00 16.03	MTGL
ATOM	1088	CB	LEU	141	44.711	11.839	33.191	1.00 14.81	MTGL
ATOM	1089	ÇG	LEU	141	44.626	10.646	32.220	1.00 15.72	MTGL
ATOM	1090	CD1	LEU	141	45.076	11.054	30.818	1.00 14.73	MTGL
MOTA	1091	CD2	LEU	141	45.494	9.501	32.752	1.00 14.97	MTGL
ATOM	1092	Ċ _	LEU	141	44.166			1.00 16.13	
ATOM	1093					12.822	35.444		MTGL
		0	LEU	141	44.776	13.819	35.069	1.00 15.77	MTGL
ATOM	1094	N	TRP	142	43.631	12.715	36.655	1.00 16.15	MTGL
ATOM	1095	CA	TRP	142	43.718	13.789	37.635	1.00 16.13	MTGL
ATOM	1096	CB	TRP	142	42.854	13.446	38.845	1.00 16.04	MTGL
ATOM	1097	CG	TRP	142	41.387	13.408	38.559	1.00 16.68	MTGL
ATOM	1098	CD2		142	40.345	13.114	39.494	1.00 16.86	
ATOM	1099	CE2		142	39.117				MTGL
						13.217	38.800	1.00 16.85	MTGL
ATOM	1100	CE3		142	40.330	12.779	40.855	1.00 17.53	MTGL
ATOM	1101	CD1	TRP	142	40.769	13.669	37.365	1.00 16.02	MTGL

Fig. 1 cont.

2001	1102	NE1	G QT	142	39.404	13.557	37.503	1.00 16.14	MTGL
ATOM	1102		TRP	142	37.884	12.993	39.421	1.00 16.71	MTGL
MOTA	1103		TRP	142	39.097	12.557	41.475	1.00 17.85	MTGL
ATOM	1104	CZ3 CH2		142	37.894	12.666	40.755	1.00 17.70	MTGL
ATOM	1105			142	45.151	14.036	38.092	1.00 16.70	MTGL
MOTA	1106	C	TRP		45.965	13.116	38.132	1.00 15.98	MTGL
MOTA	1107	0	TRP	142	45.476	15.289	38.452	1.00 18.10	MTGL
MOTA	1108	N	PRO	143	46.716	15.597	39.183	1.00 18.05	MTGL
MOTA	1109	CD	PRO	143		16.458	38.444	1.00 17.24	MTGL
MOTA	1110	CA	PRO	143	44.586	17.362	39.539	1.00 17.56	MTGL
MOTA	1111	CB	PRO	143	45.170		40.260	1.00 19.44	MTGL
MOTA	1112	CG	PRO	143	46.199	16.496	37.096	1.00 17.09	MTGL
ATOM	1113	С	PRO	143	44.599	17.177		1.00 16.74	MTGL
MOTA	1114	0	PRO	143	43.804	18.092	36.864	1.00 16.23	MTGL
ATOM	1115	N	THR	144	45.509	16.767	36.219	1.00 10.25	. MTGL
MOTA	1116	CA	THR	144	45.651	17.396	34.910		MTGL
ATOM	1117	CB	THR	144	46.677	16.640	34.048	1.00 17.49	MTGL
MOTA	1118	OG1	THR	144	47.864	16.413	34.817	1.00 18.41	MTGL
ATOM	1119	CG2	THR	144	47.040	17.453	32.811	1.00 17.61	
ATOM	1120	С	THR	144	44.346	17.510	34.129	1.00 16.98	MTGL
ATOM	1121	0	THR	144	44.027	18.579	33.610	1.00 17.37	MTGL
MOTA	1122	N	GLY	145	43.594	16.414	34.052	1.00 17.00	MTGL MTGL
ATOM	1123	CA	GLY	145	42.336	16.432	33.322	1.00 16.55	
ATOM	1124	C	GLY	145	41.111	16.472	34.219	1.00 17.19	MTGL
MOTA	1125	Ö.	GLY	145	40.033	16.013	33.837	1.00 15.11	MTGL
ATOM	1126	N	ARG	146	41.269	17.009	35.423	1.00 16.86	MTGL
ATOM	1127	CA	ARG	146	40.153	17.118	36.361	1.00 18.80	MTGL
ATOM	1128	CB	ARG	146	40.707	17.308	37.784	1.00 20.43	MTGL
MOTA	1129	CG	ARG	146	39.671	17.572	38.870	1.00 24.77	MTGL
ATOM	1130	CD	ARG	146	38.729	16.394	39.052	1.00 27.03	MTGL
ATOM	1131	NE	ARG	146	37.715	16.623	40.081	1.00 30.10	MTGL
ATOM	1132	CZ	ARG	146	37.922	16.516	41.391	1.00 31.39	MTGL
MOTA	1133		ARG	146	39.122	16.182	41.861	1.00 31.38	MTGL
	1134		ARG	146.	36.916	16.729	42.236	1.00 32.17	MTGL
ATOM	1134	C	ARG	146	39.261	18.308	35.961	1.00 18.91	MTGL
ATOM	1136	õ	ARG	146	39.763	19.344	35.534	1.00 17.30	MTGL
MOTA		И	THR	147	37.940	18.147	36.055	1.00 18.95	MTGL
ATOM	1137		THR	147	37.037	19.255	35.732	1.00 19.02	MTGL
ATOM	1138	CA	THR	147	35.550	18.826	35.731	1.00 18.33	MTGL
ATOM	1139	CB	THR	147	35.278	18.044	36.890	1.00 18.17	MTGL ·
MOTA	1140				35.217	18.016	34.490	1.00 18.17	MTGL
ATOM	1141		THR	147	37.278	20.271	36.858	1.00 19.51	MTGL
ATOM	1142	С	THR	147	37.539	19.861	37.983	1.00 18.48	MTGL
ATOM	1143	0	THR	147	37.158	21.574	36.598	1.00 19.44	MTGL
MOTA	1144	N	GLU	148		22.124	35.317	1.00 20.37	MTGL
MOTA	1145	CA	GLU	148	36.771			1.00 22.32	MTGL
MOTA	1146	CB	GLU	148	35.829			1.00 26.58	MTGL
ATOM	1147	CG	GLU	148	34.576			1.00 29.48	MTGL
MOTA	1148	CD	GLU	148	34.081	24.123		1.00 30.90	MTGL
ATOM	1149		l GLU		33.777			1.00 30.75	MTGL
MOTA	1150		2 GLU		33.988	23.929		1.00 30.73	MTGL
MOTA	1151	C	GLU		37.858				MTGL
MOTA	1152	0	GLŲ		37.649				MTGL
MOTA	1153	N	ASN		39.019				MTGL
ATOM	1154	CA	ASN		40.039				MTGL
MOTA	1155				41.436				
ATOM	1156				42.198				MTGL
ATOM	1157		1 ASN		42.651				MTGL
A'TOM	1158		2 ASN		42.298	21.917			MTGL
ATOM	1159		ASN		39.555		31.811	0.50 19.48	MTGL

Fig. 1 cont.

MOTA	1160	0	ASN	149	40.152	20.702	31.289	0.50 17.94	MTGL
MOTA	1161	N	TRP	150	38.480	22.230	31.261	1.00 19.00	MTGL
MOTA	1162	CA	TRP	150	37.920	21.769	30.000	1.00 18.91	MTGL
ATOM	1163	CB	TRP	150	36.77 <i>7</i>	22.704	29.605	1.00 18.17	MTGL
ATOM	1164	CG	TRP	150	35.710	22.781	30.629	1.00 17.82	MTGL
ATOM	1165	CD2	TRP	150	34.895	21.702	31.094	1.00 18.44	MTGL
ATOM	1166	CE2	TRP	150	34.013	22.232	32.060	1.00 18.24	MTGL
ATOM	1167	CE3		150	34.824	20.335	30.787	1.00 18.25	MTGL
ATOM	1168	CD1		150	35.301	23.895	31.310	1.00 17.99	MTGL
MOTA	1169		TRP	150	34.282	23.571	32.170	1.00 19.19	MTGL
MOTA	1170		TRP	150	33,066	21.443	32.725	1.00 19.86	MTGL
ATOM	1171		TRP	150	33.879	19.547	31.448	1.00 19.02	MTGL
MOTA	1172		TRP	150	33.013	20.105	32.408	1.00 19.52	MTGL
ATOM	1173	C	TRP	150	38.990	21.744	28.904	1.00 19.25	MTGL
ATOM	1174	0	TRP	150	39.022	20.828	28.091	1.00 19.43	MTGL
MOTA	1175	N	ALA	151	39.851	22.759	28.880	100 17.86	MTGL
ATOM	1176	CA	ALA	151	40.997	22.822	27.864	1.00 18.96	MTGL
ATOM	1177	CB	ALA	151	41.753	24.090	28.047	1.00 19.41	MTGL MTGL
ATOM	1178	C	ALA	151	41.784	21.571	27.897	1.00 18.90 1.00 19.89	MTGL
MOTA	1179	0	ALA	151	42.098	20.994	26.857	1.00 19.89	MIGL
ATOM ATOM	1180 1181	N	ASN ASN	152 152	42.184 43.027	21.144 19.954	29.088 29.209	1.00 18.43	MTGL
ATOM	1182	CA CB	ASN	152	43.584	19.830	30.635	1.00 16.07	MTGL
MOTA	1183	CG	ASN	152	44.767	20.764	30.886	1.00 18.19	MTGL
ATOM	1184		ASN	152	45.095	21.603	30.054	1.00 17.89	MTGL
ATOM	1185		ASN	152	45.407	20.618	32.043	1.00 17.33	MTGL
MOTA	1186	C	ASN	152	42.250	18.686	28.848	1.00 17.46	MTGL
ATOM	1187	ŏ	ASN	152	42.762	17.805	28.155	1.00 17.16	MTGL
ATOM	1188	N	ILE	153	41.016	18.598	29.325	1.00 17.57	MTGL
ATOM	1189	CA	ILE	153	40.177	17.437	29.048	1.00 18.34	MTGL
ATOM	1190	CB	ILE	153	38.801	17.573	29.741	1.00 17.84	MTGL
ATOM	1191		ILE	153	37.836	16.486	29.243	1.00 17.51	MTGL
ATOM	1192		ILE	153	38.987	17.468	31.255	1.00 17.49	MTGL
ATOM	1193	CD1	ILE	153	37.761	17.837	32.060	1.00 17.26	MTGL
MOTA	1194	C	ILE	153	39.974	17.246	27.548	1.00 17.82	MTGL
ATOM	1195	0	ILE	153	40.174	16.150	27.027	1.00 17.52	MTGL
ATOM	1196	N	ALA	154	39.596	18.318	26.858	1.00 17.93	MTGL
MOTA	1197	CA	ALA	154	39.359	18.255	25.416	1.00 18.68	MTGL
ATOM	1198	CB	ALA	154	38.884	19.620	24.896	1.00 17.82	MTGL
ATOM	1199	С	ALA	154	40.624	17.834	24.686	1.00 18.79	MTGL
MOTA	1200	0	ALA	154	40.584	17.037	23.744	1.00 17.95	MTGL
ATOM	1201	N	ARG	155	41.749	18.375	25.131	1.00 18.32	MTGL
ATOM	1202	CA	ARG	155	43.025	18.064	24.512	1.00 19.09	MTGL
ATOM	1203	CB	ARG	155	44.098	18.972	25.094	1.00 20.03	MTGL
MOTA	1204	CG	ARG	155	45.415	18.867	24.403	1.00 23.57	MTGL
MOTA	1205	CD	ARG	155	46.295	19.990	24.873	1.00 26.84	MTGL
ATOM	1206	NE	ARG	155	47.681	19.767	24.498	1.00 29.65	MTGL
ATOM	1207	CZ	ARG	155	48.686	20.513	24.931	1.00 28.58	MTGL
MOTA	1208		ARG	155	48.443	21.525	25.753	1.00 29.23	MTGL
ATOM	1209		ARG	155	49.922	20.244	24.540	1.00 29.12	MTGL
ATOM	1210	C	ARG	155	43.402	16.598	24.721	1.00 18.37	MTGL MTGL
MOTA MOTA	1211 1212	0	ARG	155 156	43.848	15.916	23.792	1.00 17.92	MTGL
ATOM	1212	N CA	LEU	156 156	43.540	16.115 14.731	25.944 26.258	1.00 17.77	MTGL
ATOM	1213	CB	LEU	156	43.360	14.731	27.761	1.00 17.18	MTGL
ATOM	1214	CG	LEU	156	44.375	15.158	28.689	1.00 16.00	MTGL
ATOM	1215		LEU	156	43.921	15.136	30.139	1.00 18.04	MTGL
ATOM	1217		LEU	156	45.745	14.532	28.504	1.00 17.04	MTGL
				~~~	20.770			_, _ , _ ,	

Fig. 1 cont.

ATOM	1218	С	LEU	156	42.660	13.777	25.447	1.00 17.2	9 MTGL
MOTA	1219	ŏ	LEU	156	43.152	12.794	24.886	1.00 16.7	1 MTGL
ATOM	1220	N	LEU	157	41.363	14.071	25.377	1.00 16.4	
ATOM	1221	CA	LEU	157	40.438	13.219	24.639	1.00 16.7	
MOTA	1222	СВ	LEU	157	38.992	13.651	24.900	1.00 15.2	
ATOM	1223	CG	LEU	157	38.509	13.425	26.339	1.00 14.1	
ATOM	1224	CD1		157	37.080	13.903	26.505	1.00 13.6	
MOTA	1225	CD2		157	38.599	11.944	26.676	1.00 13.6	-
ATOM	1226	C	LEU	157	40.744	13.230	23.146	1.00 18.1	
MOTA	1227	Ö	LEU	157	40.549	12.224	22.456	1.00 16.8	_
MOTA	1228	N	HIS	158	41.231	14.366	22.652	1.00 19.8	
ATOM	1229	CA	HIS	158	41.600	14.498	21.244	1,00 20.9	
ATOM	1230	CB	HIS	158	42.001	15.946	20.938	1.00 22.9	-
MOTA	1231	CG	HIS	158	42.458	16.170	19.528	1.00 24.3	
ATOM	1232		HIS	158	43.695	16.367	19.013	1.00 23.8	
ATOM	1233		HIS	158	41.586	16.230	18.460	1.00 24.9	
MOTA	1234	CE1		158	42.266	16.460	17.350	1.00 23.2	
ATOM	1235		HIS	158	43.548	16.547	17.658	1.00 24.5	
ATOM	1235	C	HIS	158	42.783	13.567	20.973	1.00 21.0	
ATOM	1237	õ	HIS	158	42.809	12.851	19.971	1.00 21.7	
ATOM	1238	N	SER	159	43.762	13.578	21.874	1.00 20.2	
ATOM	1239	CA	SER	159	44.940	12.730	21.726	1.00 20.7	
ATOM	1240	CB	SER	159	45.961	13.021	22.829	1.00 21.8	
ATOM	1241	OG	SER	159	46.476	14.333	22.721	1.00 24.7	
ATOM	1242	C	SER	159	44.570	11.253	21.774	1.00 18.9	
ATOM	1243	Ö	SER	159	45.095	10.453	21.004	1.00 19.3	
ATOM	1244	N	ALA	160	43.675	10.894	22.687	1.00 17.8	
ATOM	1245	CA	ALA	160	43.249	9.504	22.824	1.00 17.9	
ATOM	1246	CB	ALA	160	42.322	9.352	24.026	1.00 18.2	
ATOM	1247	CD	ALA	160	42.538	9.044	21.556	1.00 18.	
MOTA	1248	Ö	ALA	160	42.844	7.982	21.013	1.00 17.	
ATOM	1249	N	ALA	161	41.593	9.852	21.083	1.00 18.0	
ATOM	1250	CA	ALA	161	40.846	9.519	19.875	1.00 18.	
MOTA	1251	CB	ALA	161	39.851	10.623	19.547	1.00 16.1	
ATOM	1252	C	ALA	161	41.778	9.294	18.695	1.00 18.	
ATOM	1253	õ	ALA	161	41.654	8.301	17.983	1.00 19.	
MOTA	1254	Й	TRP	162	42.715	10.211	18.485	1.00 18.	
ATOM	1255	CA	TRP	162	43.636	10.057	17,371	1.00 19.	
ATOM	1256	CB	TRP	162	44.330	11.386	17.064	1.00 21.	
ATOM	1257	CG	TRP	162	43.420	12.264	16.268	1.00 24.0	
ATOM	1258		TRP	162	43.215	12.212	14.851	1.00 24.	
ATOM	1259	CE2		162	42.158	13.102	14.546	1.00 24.	
ATOM	1260			162	43.822	11.499	13,808	1.00 25.	
ATOM	1261		TRP	162	42.509	13.160	16.752	1.00 24.	
ATOM	1262		TRP	162	41.743	13.665	15.724	1.00 25	
ATOM	1263		TRP	162	41.691	13.293	13.241	1.00 24.	
ATOM	1264		TRP	162	43.355	11,689	12.507	1.00 25.	
ATOM	1265		TRP	162	42.302	12.581	12.238	1.00 24.	
	1266			162				1.00 20.	
ATOM	1267	õ	TRP	162	45.263	8.483	16.596	1.00 19.	
MOTA	1268	Ŋ	GLY	163	44.803	8.458	18.786	1.00 20.	
ATOM	1269	CA	GLY	163	45.703	7.343	19.016	1.00 20.	
ATOM	1270	C	GLY	163	45.051	6.124	18.375	1.00 20.	
MOTA	1271	Ö	GLY	163	45.720	5.225	17.868	1.00 20.	
ATOM	1272	И	ILE	164	43.724	6.109	18.395	1.00 20.	
ATOM	1273	ÇA	ILE	164	42.956	5.020	17.810	1.00 19.	
MOTA	1274	CB	ILE	164	41.515	5.020	18.347	1.00 18.	
ATOM	1275		ILE	164	40.670	3.977	17.601	1.00 17.	
				~ ~ 3	30.070		2.,001		

Fig. 1 cont.

MOTA	1276	CG1	ILE	164	41.529	4.750	19.852	1.00 18.11	MTGL
ATOM	1277	CD1	ILE	164	40.155	4.779	20.489	1.00 18.52	MTGL
ATOM	1278					5.181			
		C	ILE	164	42.913		16.291	1.00 20.20	MTGL
ATOM	1279	0	ILE	164	43.125	4.219	15.548	1.00 18.00	MTGL
MOTA	1280	N	LYS	165	42.645	6.405	15.839	1.00 20.30	MTGL
ATOM	1281	CA	LYS	165	42.563	6.701	14.410	1.00 21,80	MTGL
ATOM	1282	CB	LYS	165	42.100	8.149	14.191	1.00 21.88	MTGL
MOTA	1283	CG	LYS	165	40.670	8.436	14.647	1.00 23.28	MTGL
MOTA	1284	CD	LYS	165	40.346	9.924	14.509	1.00 22.94	MTGL
ATOM	1285	CE	LYS	165	38.989	10.268	15.097	1.00 24.34	MTGL
MOTA	1286	NZ	LYS	165	37.857	9.632	14.363	1.00 25.77	MTGL
MOTA	1287	С	LYS	165	43.879	6.468	13.668	1.00 21.72	MTGL
ATOM	1288	0	LYS	165	43.868	. 6,086	12.501	1.00 21.82	MTGL
ATOM	1289	N	ASP	166	45.009	6.699	14.335	1.00 22.15	MTGL
MOTA		. CA	ASP	166	46.315	6.496	13.705	1.00 21.98	MTGL
ATOM	1291	CB	ASP	166	47.373	7.438	14.299	1.00 22.61	MTGL
ATOM	1292	CG	ASP	166	47.119	8.907	13.970	1.00 24.69	MTGL
ATOM	1293		ASP	166	46.345	9.197	13.032	1.00 25.51	MTGL
	1294								
ATOM			ASP	166	47.709	9.775	14.645	1.00 23.73	MTGL
ATOM	1295	С	ASP	166	46.818	5.063	13.853	1.00 21.80	MTGL
ATOM	1296	0	ASP	166	47.900	4.737	13,373	1.00 22.35	MTGL
· MOTA	1297	N	SER	167	46.043	4.208	14.511	1.00 21.58	MTGL
ATOM	1298	CA							
			SER	167	46.460	2.822	14.722	1.00 21.57	MTGL
ATOM	1299	CB	SER	167	45.724	2.229	15.927	1.00 20.98	MTGL
ATOM	1300	OG	SER	167	44.368	1.952	15.620	1.00 20.07	MTGL
MOTA	1301	С	SER	167	46.235	1.920	13.508	1.00 21.73	MTGL
ATOM	1302	ō	SER	167	45.669	2.347	12.503	1.00 21.01	MTGL
ATOM	1303	N	SER	168	46.676	0.668	13.619	1.00 21.44	MTGL
MOTA	1304	CA	SER	168	46.520	-0.304	12.539	1.00 20.71	MTGL
ATOM	1305	CB	SER	168	47.711	-1.264	12.519	1.00 21.31	MTGL
MOTA	1306	OG	SER	168	47.836	-1.921	13.768	1.00 23.08	MTGL
ATOM	1307	Ċ	SER	168	45.229	-1.116	12.654		
								1.00 20.14	MTGL
ATOM	1308	0	SER	168	45.001	-2.033	11.869	1.00 19.79	$\mathtt{MTGL}$
ATOM.	1309	N	LEU	169	44.388	-0.792	13.630	1.00 19.27	MTGL
ATOM	1310	CA	LEU	169	43.132	-1.514	13.791	1.00 19.92	MTGL
MOTA	1311	CB	LEU	169	42.306	-0.921	14.935	1.00 19.48	MTGL
ATOM	1312	CG	LEU	169	42.758				
						-1.226	16.365	1.00 19.56	MTGL
ATOM	1313		LEU	169	41.918		17.342	1.00 18.93	MTGL
MOTA	1314	CD2	LEU	169	42.612	-2.717	16.650	1.00 19.30	MTGL
MOTA	1315	C	LEU.	169	42.323	-1.450	12.501	1.00 20.54	MTGL
ATOM	1316	0	LEU	169	42.053	-0.365	11.981	1.00 20.27	MTGL
ATOM									
	1317	Ŋ	SER	170	41.940	-2.614	11.987	1.00 20.36	MTGL
MOTA	1318	CA	SER	170	41.159	-2.678	10.760	1.00 21.47	MTGL
ATOM	1319	CB	SER	170	42.088	-2.784	9.545	1.00 22.54	MTGL
ATOM	1320	OG	SER	170	41.344	-2.749	8.341	1.00 22.78	MTGL
ATOM	1321	C	SER	170	40.216	-3.875	10.797	1.00 21.69	MTGL
MOTA	1322	0	SER	170	40.659	-5.024	10.819	1.00 21.79	MTGL
ATOM	1323	N	PRO	171	38.899	-3.621	10.800	1.00 21.30	MTGL
ATOM	1324	CD	PRO	171	37.874	-4.676	10.884	1.00 21.70	MTGL
MOTA	1325	CA	PRO	171	38.277	-2.294	10.764	1.00 21.48	MTGL
ATOM	1326	CB	PRO	171	36.806	-2.616	10.530	1.00 21.60	MTGL
ATOM	1327	CG	PRO	171	36.644	-3.901	11.285	1.00 22.67	MTGL
MOTA	1328	С	PRO	171	38.497	-1.472	12.039	1.00 21.36	MTGL
ATOM	1329	0	PRO	171	38.790	-2.009	13.109	1.00 20.24	MTGL
ATOM	1330	N	LYS	172	38.351	~0.161	11.908	1.00 20.37	MTGL
ATOM	1331	CA	LYS	172.	38.525	0.749	13.032	1.00 21.42	MTGL
MOTA	1332	CB	LYS	172	38.670	2.183	12.501	1.00 22.43	MTGL
ATOM	1333	CG	LYS	172	39.602	3.071	13.310	1.00 25.68	MTGL

Fig. 1 cont.

ATOM	1334	CD	LYS	172	41.052	2.616	13.220	1,00 24.85	MTGL
ATOM	1335	CE	LYS	172	41.659	2.946	11,878	1.00 25.80	MTGL
						2.294	11.703	1.00 24.26	MTGL
ATOM	1336	NZ	LYS	172	42.984			1.00 20.16	
MOTA	1337	С	LYS	172	37.295	0.626	13.940		MTGL .
ATOM	1338	0	LYS	172	36.199	0.307	13.478	1.00 19.92	MTGL
ATOM	1339	N	PRO	173	37.465	0.848	15.248	1.00 19.30	MTGL
ATOM	1340	CD	PRO	173	38.722	1.088	15.980	1.00 19.67	MTGL
ATOM	1341	CA	PRO	173	36.335	0.751	16.177	1,00 19.05	MTGL
ATOM	1342	CB	PRO	173	37.018	0.437	17,497	1.00 19.14	MTGL
						1.321	17.412	1.00 18.48	MTGL
ATOM	1343	CG	PRO	173	38.237			1.00 18.59	
ATOM	1344	C	PRO	173	35.565	2.066	16.270		. MTGL
MOTA	1345	0	PRO	173	36.049	3.110	15.832	1.00 16.92	MTGL
MOTA	1346	N	LYS	174	34.359	2.007	16.624	1.00 17.93	MTGL
ATOM	1347	CA	LYS	174	33.591	3.222	17.037	1.00 18.70	MTGL
ATOM	1348	CB	LYS	174	32.109	2.901	17.240	1.00 18.25	MTGL
ATOM	1349	CG	LYS	174	31.388	2.529	15.947.	1.00 19.90	MTGL
ATOM	1350	CD	LYS	174	29.937	2.142	16.200	1.00 20.92	MTGL
						1.784	14.892	1.00 21.51	MTGL
ATOM	1351	CE	LYS	174	29.230				
ATOM	1352	NZ	LYS	174	27.839	1.317	15.135	1.00 20.89	MTGL
MOTA	1353	С	LYS	174	34.193	3.808	18.318	1.00 18.48	MTGL
ATOM	1354	0	LYS	174	34.452	3.076	19.281	1.00 18.00	$\mathtt{MTGL}$
MOTA	1355	N	ILE	175	34.448	5.112	18.320	1.00 17.76	MTGL
ATOM	1356	CA	ILE	175	35.033	5.768	19.487	1.00 17.60	MTGL
ATOM	1357	СВ	ILE	175	35.999	6.883	19.050	1.00 17.54	MTGL
ATOM	1358	CG2	ILE	175	36.564	7.610	20.271	1.00 17.48	MTGL
ATOM			ILE			6.266	18.226	1.00 16.88	MTGL
	1359	CG1		175	37.134				
ATOM	1360	CD1	ILE	175	38.083	7.263	17.618	1.00 15.96	MTGL .
MOTA	1361	С	ILE	175	33.945	6.330	20.393	1.00 17.11	MTGL
MOTA	1362	0	ILE	175	33.102	7.122	19.962	1.00 17.92	MTGL
ATOM	1363	N	MET	176	33.966	5.914	21.653	1.00 16.13	MTGL
ATOM	1364	CA	MET	176	32.955	6.345	22.615	1.00 16.14	MTGL
ATOM	1365	CB	MET	176	32.223	5.120	23.171	1.00 16.50	MTGL
ATOM	1366	CG	MET	176	31.333	5.410	24.379	1.00 16.70	MTGL
ATOM	1367	SD	MET	176	30.643	3.896	25.097	1.00 19.61	MTGL
	1368	CE	MET	176	29.473	3.433	23.769	1.00 15.01	MTGL
MOTA									MTGL
ATOM	1369	c	MET	176	33.458	7.163	23.797	1.00 16.18	
ATOM	1370	0	MET	176	34.562	6.946	24.299	1.00 15.62	MTGL
MOTA	1371	N	ILE	177	32.628	8.109	24.227	1.00 16.05	MTGL
ATOM	1372	CA	ILE	177	32.915	8.927	25.402	1.00 16.22	MTGL
MOTA	1373	CB	ILE	177	32.786	10.436	25.117	1.00 15.59	mtgl
ATOM	1374	CG2	ILE	177	32.729	11.210	26.438	1.00 16.50	MTGL
ATOM	1375		ILE	177	33.985	10.900	24.273	1.00 16.91	MTGL
ATOM	1376		ILE	177	33.988	12.380	23.935	1.00 17.23	MTGL
ATOM	1377	C	ILE	177	31.847	8.467	26.383	1.00 15.72	MTGL
								1.00 16.21	MTGL
ATOM	1378	0	ILE	177	30.660	8.467	26.062		
ATOM	1379	N	HIS	178	32.278	8.061	27.571	1.00 16.15	MTGL
MOTA	1380	CA	HIS	178	31.376	7.518	28.581	1.00 16.02	MTGL
ATOM	1381	CB	HIS	178	31.866	6.112	28.949	1.00 14.76	MTGL
MOTA	1382	CG	HIS	178	31.099	5.461	30.057	1.00 14.66	MTGL
ATOM	1383		HIS	178	29.850	5.681	30.534	1.00 13.15	MTGL
ATOM	1384		HIS	178	31.612	4.415	30.793	1.00 13.39	MTGL
ATOM	1385		HIS	178	30.714	4.020	31.679	1.00 14.18	MTGL
						4.770	31.543	1.00 13.19	MTGL
ATOM	1386		HIS	178	29.636				
ATOM	1387	C	HIS	178	31.232	8.354	29.850	1.00 16.83	MTGL
ATOM	1388	0	HIS	178	32.210	8.605	30.553	1.00 16.59	MTGL
MOTA	1389	N	<b>LEU</b>	179	29.997	8.757	30.138	1.00 17.26	MTGL
ATOM	1390	CA	LEU	179	29.670	9.539	31.329	1.00 18.11	$\mathtt{MTGL}$
MOTA	1391	CB	ΓEΩ	179	29.014	10.866	30.925	1.00 18.73	$\mathtt{MTGL}$

Fig. 1 cont.

ATOM	1392	CG	LEU	179	29.877	12.128	30.808	1.00 20.65	MTGL
ATOM	1393	CDI	LEU	179	31.265	11.812	30.272	1.00 19.45	MTGL
ATOM	1394	CD2	LEU	179	29.150	13.130	29.923	1.00 20.83	MTGL
ATOM	1395	С	LEU	179	28.693	8.732	32.186	1.00 18.96	MTGL
ATOM	1396	0	LEU	179	27.947	7.899	31.668	1.00 19.30	MTGL
ATOM	1397	N	ASP	180	28.693	8.974	33.493	1.00 18.24	MTGL
ATOM	1398	CA	ASP	180	27.780	8.267	34.385	1.00 18.02	MTGL
MOTA	1399	CB	ASP	180	28.377	8.171	35.795	1.00 17.69	MTGL
ATOM	1400	CG	ASP	180	28.398	9.505	36.518	1.00 19.25	MTGL
MOTA	1401		ASP	180	28.702	10.538	35.884	1.00 19.57	MTGL
ATOM	1402	OD2	ASP	180	28.117	9.512	37.734	1.00 20.92	MTGL
ATOM	1403	С	ASP	180	26.453	9.020	34.430	1.00 18.13	MTGL
MOTA	1404	0	ASP	180	26.268	9.995	33.708	1.00 17.92	MTGL
ATOM	1405	N	ASN	181	25.533	8.546	35.266	1.00 19.02	MTGL
ATOM	1406	CA	ASN	181	24.219	9.165	35.439	1.00 19.13	MTGL
	_								
MOTA	1407	CB	ASN	181	24.337	10.360	36.393	1.00 19.61	MTGL
ATOM	1408	ĊG	ASN	181	24.840	9.959	37.776	1.00 20.81	MTGL
ATOM	1409	OD1	ASN	181	24.561	8.857	38.259	1.00 20.36	MTGL
ATOM	1410		ASN	181	25.567	10.862	38.427	1.00 21.46	$\mathtt{MTGL}$
ATOM	1411	С	ASN	181	23.541	9.604	34.135	1.00 19.21	MTGL
ATOM	1412	0	ASN	181	23.277	10.791	33.925	1.00 18.32	MTGL
MOTA	1413	Ŋ	GLY	182	23.238	8.635	33.276	1.00 18.94	MTGL
ATOM	1414	CA	$\mathbf{G}\mathbf{F}\mathbf{A}$	182	22.610	8.937	32.003	1.00 18.55	MTGL
ATOM	1415	С	GLY	182	21.309	9.704	32.101	1.00 18.91	MTGL
MOTA	1416	0	GLY	182	20.952	10.428	31.179	1.00 18.95	$\mathtt{MTGL}$
MOTA	1417	N	TRP	183	20.609	9.546	33.219	1.00 19.65	MTGL
ATOM	1418	CA	TRP	183	19.332	10.213	33.459	1.00 19.57	MTGL
		_							
ATOM	1419	CB	TRP	183	18.643	9.588	34.671	1.00 20.28	MTGL
MOTA	1420	CG	TRP	183	19.515	9.586	35.904	1.00 21.43	MTGL
ATOM	1421	CD2	TRP	183	19.671	10.653	36.856	1.00 21.48	MTGL
MOTA	1422	CE2	TRP	183	20.614	10.222	37.816	1.00 21.25	MTGL
MOTA	1423	CE3	TRP	183	19.103	11.931	36.989	1.00 21.53	MTGL
ATOM	1424	CD3	TRP	183	20.348	8.585	36.316	1.00 20.88	MTGL
ATOM	1425		TRP	183	21.011	8.959	37.463	1.00 21.48	MTGL
MOTA	1426	CZ2	TRP	183	21.010	11.024	38.896	1.00 22.46	$\mathtt{MTGL}$
ATOM	1427	CZ3	TRP	183	19,497	12.732	38.065	1.00 21.36	MTGL
	1428								
ATOM			TRP	183	20.440	12.272	39.004	1.00 21.87	MTGL
ATOM	1429	С	TRP	183	19.477	11.705	33.724	1.00 20.04	MTGL
ATOM	1430	0	TRP	183	18.506	12.457	33.613	1.00 19.18	MTGL
ATOM	1431	N	ASP	184	20.686				
						12.126	34.083	1.00 20.76	MTGL
ATOM	1432	CA	ASP	184	20.957	13.522	34.417	1.00 20.14	MTGL
ATOM	1433	CB	ASP	184	22.085	13.581	35.455	1.00 21.31	MTGL
ATOM	1434	CG	ASP	184	22.327	14.986	35.988	1.00 24.62	MTGL
ATOM	1435	ODI	ASP	184	21.643	15.936	35.540	1.00 24.90	MTGL
MOTA	1436	OD2	ASP	184	23.210	15.138	36.859	1.00 25.79	MTGL
ATOM	1437	Ċ	ASP	184	21.312	14.374	33.201	1.00 20.22	MTGL
ATOM	1438	Q	ASP	184	22.487	14.584	32.899	1.00 19.35	MTGL
MOTA	1439	N	TRP	185	20.289	14.879	32.518	1.00 19.30	$\mathtt{MTGL}$
ATOM	1440	CA	TRP						
				185		15.704	31.333	1.00 19.09	MTGL
ATOM	1441	CB	TRP	185	19.148	16.149	30.753	1.00 18.81	MTGL
ATOM	1442	CG	TRP	185	19.267	17.255	29.746	1.00 18.32	MTGL
ATOM	1443		TRP	185	20.044	17.245	28.541	1.00 18.10	MTGL
ATOM	1444		TRP	185	19.889	18.509	27.933	1.00 18.68	MTGL
ATOM	1445	CE3	TRP	185	20.856	16.290	27.917	1.00 18.54	MTGL
ATOM	1446		TRP	185					
					18.686	18.491	29.814	1.00 18.71	MTGL
MOTA	1447		TRP	185	19.057	19.250	28.730	1.00 18.49	MTGL
ATOM	1448	CZ2	TRP	185	20.518	18.845	26.732	1.00 19.18	MTGL
MOTA	1449		TRP	185	21.484	16.626	26.722	1.00 18.13	MTGL
				-00	307	10.020	~~, ,		111011

Fig. 1 cont.

ATOM	1450	CH2	TRP	185	21.311	17.891	26.144	1.00 19.60	MTGL
					21.360	16.931	31.626	1.00 18.76	MTGL
ATOM	1451	С	TRP	185					
MOTA	1452	0	$\mathtt{TRP}$	185	22.271	17.256	30.866	1.00 17.61	MTGL
ATOM	1453	N	GLY	186	21.068	17.612	32.731	1.00 19.33	MTGL
MOTA	1454	CA	GLY	186	21.834	18.797	33.081	1.00 19.04	MTGL
ATOM	1455	С	GLY	186	23.336	18.565	33.066	1.00 19.17	MTGL
ATOM	1456	0	GLY	186	24.098	19.353	32.505	1.00 19.02	MTGL
ATOM	1457		THR	187	23,772	17.473	33.677	1.00 19.36	MTGL
		N							
ATOM	1458	CA	THR	187	25.192	17.172	33.718	1.00 20.31	MTGL
ATOM	1459	CB	THR	187	25.482	16,098	34.773	1.00 21.41	MTGL
ATOM	1460		THR	187	25.114	16,609	36.059	1.00 21.37	MTGL
ATOM	1461	CG2	THR	187	26.964	15.735	34.781	1.00 23.08	MTGL
ATOM ·	1462	С	THR	187	25.731	16.745	32.359	1.00 19.27	· MTGL
ATOM	1463	0	THR	187	26.815	17.166	31.965	1.00 19.21	MTGL
ATOM	1464	N	GLN	188	24.980	15.916	31.637	1.00 19.95	MTGL
MOTA	1465	CA	GLN	188	25.420	15.479	30.312	1.00 19.24	$\mathtt{MTGL}$
ATOM	1466	CB	GLN	188	24.356	14.602	29.638	1.00 19.13	MTGL
						13.278	30.329	1.00 18.75	MTGL
ATOM	1467	CG	GLN	188	24.033				
ATOM	1468	CD	GLN	188	25.203	12.299	30.339	1.00 18.38	MTGL
ATOM ·	1469	OE1	GLN	188	25.874	12.099	29.328	1.00 18.47	MTGL
ATOM	1470	NE2	GLN	188	25.435	11.675	31.483	1.00 16.34	MTGL
ATOM	1471	C	GLN	188	25.655	16.714	29.437	1.00 19.43	MTGL
MOTA	1472	0	GLN	188	26.695	16.850	28.792	1.00 18.38	MTGL ·
ATOM	1473	N	ASN	189	24,673	17.612	29.429	1.00 20.01	MTGL
									MTGL
MOTA	1474	CA	ASN	189	24.733	18.830	28.625	1,00 20.84	
MOTA	1475	CB	ASN	189	23.392	19.568	28.722	1,00 22,61	$\mathtt{MTGL}$
MOTA	1476	CG	ASN	189	23.323	20.781	27.813	1.00 24.36	MTGL
ATOM `	1477		ASN	189	23.788	20.744	26,674	1.00 24.74	MTGL
ATOM	1478	ND2	ASN	18 <del>9</del>	22.725	21.860	28.310	1.00 24.46	MTGL
ATOM	1479	С	ASN	189	25.978	19.746	29.050	1.00 21.20	$\mathtt{MTGL}$
ATOM	1480	0	ASN	189	26.622	20.267	28.214	1.00 20.76	MTGL
									MTGL
ATOM	1481	Ŋ	TRP	190	26.015	19.935	30.356	1.00 21.74	
ATOM	1482	CA	TRP	190	27.073	20.770	30.917	1.00 22.16	MTGL
ATOM	1483	CB	TRP	190	26.959	20.758	32.442	1.00 23.20	MTGL
ATOM	1484	ĊĠ	TRP	190	28.143	21.315	33.192	1.00 25.19	MTGL
ATOM	1485		TRP	190	29.121	20.563	33.925	1.00 25.40	MTGL
ATOM	1486	CE2	TRP	190	30.015	21.491	34.505	1.00 25.48	MTGL
MOTA	1487		TRP	190	29.336	19.194	34.137	1.00 25.81	MTGL
								1.00 24.81	MTGL
ATOM	1488		TRP	190	28.474	22.632	33.355		
ATOM	1489	NE1	TRP	190	29.595	22.744	34.146	1.00 26.35	MTGL
ATOM	1490	CZ2	TRP	190	31.098	21.095	35.298	1.00 26.43	MTGL
ATOM	1491		TRP	190	30.420	18,800	34.925	1.00 26.45	MTGL
								-	
ATOM	1492		TRP	190	31.288	19.750	35.490	1.00 25.29	MTGL
MOTA	1493	С	TRP	190	28.451	20.252	30.493	1.00 21.86	MTGL
ATOM	1494	0	TRP	190	29.322	21.023	30.081	1.00 21.57	MTGL
							30.586	1.00 20.42	MTGL
ATOM	1495	N	TRP	191	28.637	18.939			
MOTA	1496	CA	TRP	191	29.915	18.325	30.245	1.00 19.96	MTGL
MOTA	1497	CB	TRP	191	29.902	16.846	30.631	1.00 18.89	MTGL
ATOM	1498		TRP	191	31.272	16.231	30.703	1.00 18.14	MTGL
		CG							
MOTA	1499		TRP	191	32.017	15.658	29.621	1.00 17.74	MTGL
ATOM	1500	CE2	TRP	191	33.244	15.201	30.154	1.00 17.14	MTGL
ATOM	1501		TRP	191	31.767	15.481	28.253	1.00 17.05	MTGL
ATOM	1502		TRP	191	32.058	16.108	31.815	1.00 18.47	MTGL
ATOM	1503	NE1	TRP	191	33.241	15.489	31.494	1.00 16.67	MTGL
ATOM	1504	CZ2	TRP	191	34.221	14.583	29.366	1.00 16.52	MTGL
								1.00 15.97	MTGL
ATOM	1505		TRP	191	32.739	14.862	27.468		
ATOM	1506	CH2	TRP	191	33.950	14.420	28.030	1.00 16.29	MTGL
MOTA	1507	С	TRP	191	30.293	18.455	28.770	1.00 19.44	MTGL
		-							

Fig. 1 cont.

ATOM	1508	0	TRP	191	31.342	19.019	28,436	1.00 18.48	MTGL
ATOM	1509	N	TYR	192	29.447	17.921	27.893	1.00 19.02	MTGL
ATOM	1510	CA.	TYR	192	29.707	17.961	26.455	1.00 18.88	MTGL
ATOM	1511	CB	TYR	192	28,629	17.174	25.702	1.00 18.06	MTGL
				192			25.779	1.00 17.74	MTGL
ATOM	1512	CG	TYR		28.820	15.670			
ATOM	1513	CD1		192	29.890	15.048	25,126	1.00 17.96	MTGL
ATOM	1514	CE1	TYR	192	30.069	13.671	25.189	1.00 18.35	MTGL
ATOM	1515		TYR	192	27.935	14.870	26.502	1.00 16.89	MTGL
ATOM	1516	CE2	TYR	192	28.107	13.487	26.574	1.00 17.96	MTGL
ATOM	1517	CZ	TYR	192	29.172	12.895	25.917	1.00 18.14	MTGL
ATOM	1518	OH	TYR	192	29.340	11.530	25.986	1.00 19.50	MTGL
ATOM	1519	C	TYR	192	29.810	19.378	25.895	1.00 19.64	MTGL
ATOM	1520	0	TYR	192	30.661	19.651	25.047	1.00 17.67	MTGL
ATOM	1521	N	THR	193	28.956	20.280	26.373	1.00 20.13	MTGL
MOTA	1522	CA	THR	193	28.988	21.658	25.904	1.00 21.63	MTGL
ATOM	1523	СВ	THR	193	27.884	22.504	26.569	1.00 21.95	MTGL
ATOM	1524	OG1	THR	193	26.600	21.990	26.195	1.00 23.39	MTGL
ATOM	1525	CG2	THR	193	27.978	23.956	26.114	1.00 23.15	MTGL
ATOM	1526	C	THR	193	30.346	22.306	26.189	1.00 21.54	MTGL
ATOM	1527			193					MTGL
		0	THR		30.978	22.863	25.291	1.00 21.18	
ATOM	1528	N	ASN	194	30.804	22.218	27.434	1.00 21.85	
ATOM	1529	CA	ASN	194	32.084	22.816	27.800	1.00 22.13	MTGL
ATOM	1530	CB	ASN	194	32.243	22.833	29.318	1.00 23.00	MTGL
MOTA	1531	CG	ASN	194	31.437	23.944	29.968	1.00 24.26	MTGL '
MOTA	1532		ASN	194	31.675	25.123	29.709	1.00 25.08	MTGL
ATOM	1533	ND2	ASN	194	30.478	23.573	30.810	1.00 23.61	MTGL
MOTA	1534	С	ASN	194	33.292	22.146	27.156	1.00 21.45	MTGL
ATOM	1535	0	ASN	194	34.266	22.813	26.815	1.00 21.18	MTGL
ATOM	1536	N	VAL	195	33.236	20.831	26.986	1.00 21.36	MTGL
ATOM	1537	CA	VAL	195	34.346	20.123	26.362	1.00 20.65	MTGL
ATOM	1538	CB	VAL	195	34.187	18.590	26.503	1.00 20.76	MTGL
MOTA	1539		VAL	195	35.165	17.871	25.583	1.00 19.43	MTGL
ATOM	1540	CG2		195	34.429	18.179	27,947	1.00 20.62	MTGL
ATOM	1541	C	VAL	195	34.453	20.475	24.879	1.00 21.44	MTGL
ATOM	1542	ŏ	VAL	195	35.540	20.792	24.385	1.00 20.78	MTGL
ATOM	1543	N	LEU	196	33.323	20.429	24.178	1.00 21.29	MTGL
MOTA	1544	CA	LEU	196					
					33.300	20.712	22.746	1.00 23.23	MTGL
MOTA	1545	CB	LEU	196	31.953	20.285	22.150	1.00 22.71	MTGL
ATOM	1546	CG	LEU	196	31.703	18.772	22.118	1.00 24.14	MTGL
ATOM	1547		LEU	196	30.276	18.477	21.657	1.00 22.72	MTGL
ATOM	1548		TEO	196	32.720	18.115	21.187	1.00 23.15	MTGL
MOTA	1549	С	<b>LEO</b>	196	33.589	22.158	22.354	1.00 24.05	MTGL
MOTA	1550	0	LEU	196	34.054	22.413	21.250	1.00 24.38	MTGL
ATOM	1551	N	LYS	197	33.326	23.104	23.248	1.00 25.84	MTGL
MOTA	1552	CA	LYS	197	33.562	24.506	22.919	1.00 27.64	MTGL
ATOM	1553	CB	LYS	197	32.753	25.413	23.850	1.00 29.58	MTGL
MOTA	1554	CG	LYS	197	33.282	25.505	25.268	1.00 32.86	MTGL
MOTA	1555	CD	LYS	197	32.239	26.101	26.207	1.00 35.16	MTGL
ATOM	1556	CE	LYS	197	31.742	27.456	25.726	1.00 37.48	MTGL
ATOM	1557	NZ	LYS	197	30.672	28.001	26.617	1.00 39.55	MTGL
ATOM	1558	С	LYS	197	35.038	24.897	22.956	1.00 27.59	MTGL
ATOM	1559	ŏ	LYS	197	35.397	26.010	22.577	1.00 27.09	MTGL
ATOM	1560	N	GLN	198	35.896	23.980	23.395	1.00 27.10	MTGL
ATOM	1561	CA	GLN	198	37.323	24.271		1.00 27.10	MTGL
							23.459		
MOTA	1562	CB	GLN	198	3B.053	23.202	24.274	1.00 26.22	MTGL
ATOM	1563	CG	GLN	198	37.608	23.127	25.718	1.00 24.93	MTGL
MOTA	1564	CD	GLN	198	37.637	24.480	26.400	1.00 25.72	MTGL
MOTA	1565	OE1	GLN	198	38.667	25.152	26.432	1.00 25.49	MTGL

Fig. 1 cont.

MOTA	1566	NE2	GLN	198	36.501	24.886	26.950	1.00 24.69	MTGL
MOTA	1567	С	GLN	198	37.953	24.381	22.071	1.00 27.46	MTGL
ATOM	1568	ō	GLN	198 ·	38.937	25.097	21.885	1.00 27.60	MTGL
ATOM	1569	Ň	GLY	199	37.401	23.664	21.101	1.00 27.40.	MTGL
MOTA	1570	CA	GLY	199	37.941	23.738	19.757	1.00 28.72	MTGL
			GLY	199	39.002	22.713	19.397	1.00 29.03	MTGL
MOTA	1571	C		199	39.487	22.711	18.269	1.00 30.82	MTGL
ATOM	1572	0	GLY			21.852	20.337	1.00 27.35	MTGL
MOTA	1573	N	THR	200	39.382			1.00 26.65	MTGL
ATOM	1574	CA	THR	200	40.377	20.823	20.041		
ATOM	1575	CB	THR	200	41.335	20.596	21.230	1.00 26.55	MTGL
ATOM	1576	OG1	THR	200	40.579	20.447	22.438	1.00 27.05	MTGL
ATOM	1577	CG2	THR	200	42.297	21.780	21.366	1.00 26.96	MTGL
ATOM	1578	С	THR	200	39.633	19.532	19.705	1.00 25.68	MTGL
ATOM	1579	0	THR	200	39.665	19.072	18.569	1.00 25.00	MTGL
ATOM	1580	N	LEU	201	38.960	18,947	20.690	1.00 25.02	MTGL
ATOM	1581	CA	LEU	201	38.180	17.745	20.428	1.00 24.16	MTGL
ATOM	1582	CB	LEU	201	37.701	17.105	21.734	1.00 23.23	MTGL
				201	36.814	15.867	21.556	1.00 23.41	MTGL
ATOM	1583	CG	LEU		37.674	14.680	21.136	1.00 22.70	MTGL
MOTA	1584	CD1		201				1.00 23.70	MTGL
MOTA	1585	CD2		201	36.099	15.552	22.852		MTGL
MOTA	1586	C	LEU	201	36.967	18.221	19.628	1.00 23.81	
MOTA	1587	О.	LEU	201	36.280	19.152	20.041	1.00 22.98	MTGL
MOTA	1588	N	GLU	202	36.710	17.608	18.480	1.00 23.89	MTGL
MOTA	1589	CA	GLU	202	35.554	18.002	17.672	1.00 25.20	$\mathtt{MTGL}$
ATOM	1590	CB	GLU	202	35.962	18.281	16.227	1.00 26.99	MTGL
ATOM	1591	CG	GLU	202	37.142	19.208	16.054	1.00 30.89	` MTGL
ATOM	1592	CD	GLU	202	37.380	19.539	14.596	1.00 33.28	MTGL
ATOM	1593	OE1		202	36,601	20.338	14.034	1.00 35.02	MTGL
ATOM	1594	OE2		202	38.333	18.989	14.004	1.00 34.29	MTGL
	1595		GLU	202	34.545	16.863	17.667	1.00 24.61	MTGL
MOTA		C		202	34.886	15.725	17.990	1.00 23.46	MTGL
ATOM	1596	0	GLU				17.286	1.00 24.45	MTGL
ATOM	1597	Ŋ	LEU	203	33.311	17.169			
MOTA	1598	CA	<b>TE</b> O	203	32.267	16.157	17.222	1.00 25.47	MTGL
ATOM	1599	CB	LEU	203	30.959	16.768	16.721	1.00 26.23	MTGL
MOTA	1600	CG	LEU	203	30.009	17.289	17.794	1.00 27.61	MTGL
MOTA	1601	CD1	LEU	203	28.830	17.970	17.126	1.00 28.79	MTGL
ATOM	1602	CD2	LEU	203	29.532	16.139	18.672	1.00 27.38	MTGL
ATOM	1603	C	LEU	203	32.666	15.007	16.305	1.00 25.18	$\mathtt{MTGL}$
ATOM	1604	Õ	LEU	203	32.307	13.857	16.555	1.00 25.60	MTGL
ATOM	1605	Ň	SER	204	33.411	15.318	15.249	1.00 23.52	MTGL
ATOM	1606	CA	SER	204	33.841	14.295	14.305	1.00 23.46	MTGL
ATOM	1607	CB	SER	204	34.367	14.941	13.016	1.00 24.47	MTGL
ATOM	1608	OG	SER	204	35.559	15.677	13.253	1.00 23.17	MTGL
						13.379	14.877	1.00 22.84	MTGL
ATOM	1609	C	SER	204	34.918		14.278	1.00 22.80	MTGL
ATOM	1610	0	SER	204	35.235	12.353			
ATOM	1611	N	ASP	205	35.482	13.742	16.027	1.00 21.73	MTGL
MOTA	1612	CA	ASP	205	36.529	12.920	16.626	1.00 21.47	MTGL
ATOM	1613	CB	ASP	205	37.369	13.735	17.616	1.00 21.78	MTGL
ATOM	1614	ÇG	ASP	205	38.284	14.737	16.925	1.00 23.69	MTGL
MOTA	1615		ASP	205	38.859	14.388	15.870	1.00 23.46	MTGL
ATOM	1616		ASP	205	38.442	15.866	17.446	1.00 23.01	MTGL
ATOM	1617	C	ASP	205	36.020	11.653	17.310	1.00 20.42	MTGL
MOTA	1618	Ö	ASP	205	36.795	10.727	17.545	1.00 20.47	MTGL
		N	PHE	205	34.736	11,609	17.650	1.00 19.52	MTGL
MOTA	1619						18.275	1.00 20.33	MTGL
MOTA	1620	CA	PHE	206	34.183	10.408		1.00 20.33	MTGL
MOTA	1621	CB	PHE	206	34.060	10.565	19.801		
ATOM	1622	CG	PHE	206	33.098	11.626	20.244	1.00 18.95	MTGL
ATOM	1623	CD1	PHE	206	33.403	12.974	20.083	1.00 18.40	MTGL

Fig. 1 cont.

MOTA	1624	CD2	PHE	206	31.899	11.275	20.861	1.00 18.16	MTGL
ATOM	1625	CEI	PHE	206	32.529	13.959	20.534	1.00 19.01	MTGL
MOTA	1626	CE2	PHE	206	31.015	12.253	21.316	1.00 19.53	$\mathtt{MTGL}$
ATOM	1627	CZ	PHE	206	31.331	13.601	21,153	1.00 18.89	MTGL
ATOM	1628	С	PHE	206	32.850	10.031	17.642	1.00 20.83	MTGL
	-								
MOTA	1629	0	BHE	206	32.267	10.825	16.901	1.00 20.91	MTGL
MOTA	1630	N	ASP	207	32.365	8.827	17.937	1.00 20.94	$\mathtt{MTGL}$
ATOM	1631	CA	ASP	207	31.134	8.331	17.322	1.00 21.05	MTGL
ATOM		•							
	1632	CB	ASP	207	31.470	7.084	16.500	1.00 21.79	MTGL
ATOM	1633	CG	ASP	207	32.766	7.235	15.730	1.00 22.83	MTGL
MOTA	1634	OD1	ASP	207	32.811	8.093	14.826	1.00 22.13	MTGL
ATOM	1635		ASP	207	33.739	6.506	16.036	1.00 21.38	MTGL
ATOM	1636	C	asp	207	29.978	7.990	18.256	1.00 20.40	MTGL
MOTA	1637	0	ASP	207	28.813	8.022	17.847	1.00 20.09	MTGL
ATOM	1638	N	MET	208	30.286	7.660	19,502	1.00 19.17	MTGL
ATOM	1639	CA		208		7.281			
			MET		29.236		20.431	1.00 17.84	MTGL
ATOM	1640	CB	MET	208	29.282	5.771	20.688	1.00 17.36	MTGL
ATOM	1641	CG	MET	208	29.319	4.900	19.455	1.00 17.72	MTGL
MOTA	1642	SD	MET	208	29.434	3.141	19.906	1.00 19.72	MTGL
		-							
ATOM	1643	CE	MET	208	27.745	2.786	20.301	1.00 18.67	MTGL
ATOM	1644	С	MET	208	29.293	7.979	21,775	1.00 17.33	MTGL
ATOM	1645	0	MET	208	30.351	8.410	22.232	1.00 16.75	MTGL
ATOM	1646	N	MET	209	28.125				
						8.080	22.397	1.00 16.30	MTGL
MOTA	1647	CA	MET	209	27.991	8.653	23.722	1.00 17.25	MTGL
ATOM	1648	CB	MET	209	27.037	9.852	23.730	1.00 16.86	MTGL
ATOM	1649	CG	MET	209	27.525	11.048	22.926	1.00 17.20	MTGL
ATOM	1650	_							
		SD	MET	209	26.439	12.511	23.096	1.00 15.98	MTGL
ATOM	1651	CE	MET	209	27.636	13.808	22.762	1.00 17.32	$\mathtt{MTGL}$
ATOM	1652	С	MET	209	27.405	7.529	24.557	1.00 16.92	MTGL
ATOM	1653	0	MET	209	26,311	7.033	24.273	1.00 16.52	MTGL
ATOM	1654	N	GLY	210	28.153	7.103	25.565	1.00 16.49	MTGL
MOTA	1655	CA	GLY	210	27.675	6.038	26.423	1.00 16.81	MTGL
ATOM	1656	Ç	GLY	210	27.361	6.585	27.797	1.00 16.14	MTGL
ATOM	1657	Õ	GLY	210	27.991	7.537	28.257	1.00 15.66	
									MTGL
ATOM	1658	N	VAL	211	26.370	5.998	28.450	1.00 16.46	MTGL
ATOM	1659	CA	VAL	211	25.999	6.431	29.784	1.00 15.55	MTGL
MOTA	1660	CB	VAL	211 ·	24.691	7.247	29.773	1.00 15.54	MTGL
ATOM	1661		VAL	211	24.824	8,449	28.839	1.00 16.27	MTGL
ATOM	1662		VAL	211	23.525	. 6.354	29.353	1.00 14.06	MTGL
ATOM	1663	С	VAL	211	25.781	5.236	30.700	1.00 16.00	MTGL
ATOM	1664	0	VAL	211	25.418	4.148	30.243	1.00 15.69	MTGL
MOTA	1665	N	SER	212	26.013	5.445	31.991	1.00 15.22	MTGL
ATOM	1666	CA	SER	212	25.766	4.414	32.983	1.00 15.39	MTGL
ATOM	1667	CB	SER	212	26.741	4.537	34.158	1.00 15.48	MTGL
ATOM	1668	OG	SER	212	28.083	4.327	33.748	1.00 16.02	MTGL
ATOM	1669	C	SER	212	24.346	4.707		1.00 15.93	
							33.469		MTGL
MOTA	1670	O	SER	212	23.922	5.863	33.498	1.00 16.20	MTGL
MOTA	1671	N	PHE	213	23.599	3.670	33.821	1.00 15.04	MTGL
ATOM	1672	CA	PHE	213	22.248	3.866	34.323	1.00 15.18	MTGL
						3.000			
ATOM	1673	CB	PHE	213	21.218	3.762	33.191	1.00 14.75	MTGL
ATOM	1674	CG	PHE	213	19.801	3.982	33.647	1.00 14.40	MTGL
ATOM	1675	CD1	PHE	213	19.383	5.238	34.071	1.00 15.35	MTGL
ATOM	1676	CD2		213	18.897	2.924	33.694	1.00 14.80	MTGL
ATOM	1677	CE1		213	18.079	5.441	34.542	1.00 15.59	MTGL
MOTA	1678	CE2	PHE	213	17.594	3.113	34.160	1.00 15.14	MTGL
ATOM	1679	CZ	PHE	213	17.185	4.376	34.586	1.00 15.11	MTGL
ATOM	1680	C	PHE		21.956				
				213		2.821	35.388	1.00 16.01	MTGL
ATOM	1681	0	BHE	213	21.757	1.646	35.078	1.00 16.44	MTGL

Fig. 1 cont.

MOTA	1682	N	TYR	214	21.954	3.258	36.644	1.00 16.44	MTGL
ATOM	1683	CA	TYR	214	21.691	2.382	37.782	1.00 16.37	MTGL
ATOM	1684	CB	TYR	214	22.917	2.332	38.700	1.00 16.76	MTGL
ATOM	1685	CG	TYR	214	24.097	1.562	38,131	1.00 16.18	MTGL
MOTA	1686		TYR	214	24.114	0.168	38.139	1.00 16.62	MTGL
MOTA	1687		TYR	214	25.201	-0.544	37.637	1.00 17.99	MTGL
ATOM	1688	CD2	TYR	214	25.199	2.228	37.599	1.00 16.40	MTGL
ATOM	1689		TYR	214	26.295	1.524	37.093	1.00 16.27	MTGL
ATOM	1690	CZ	TYR	214	26.288	0.142	37.118	1.00 16.37	MTGL
MOTA	1691	ОН	TYR	214	27.375	-0.556	36.648	1.00 17.15	MTGL
MOTA	1692	C	TYR	214	20.479	2.904	38.554	1.00 17.45	MTGL
ATOM	1693	0	TYR	214	20.246	4.111	38.632	1.00 17.08	MTGL
ATOM	1694	И	PRO	215	19.691	1.997	39.140	1.00 17.07 1.00 17.36	MTGL
MOTA	1695	CD	PRO	215 215	19.704 18.506	0.537 2.395	38.916 39.896	1.00 17.38	MTGL MTGL
ATOM ATOM	1696	CA	PRO	215	17.547	1.247	39.619	1.00 17.11	MTGL
ATOM	1697 1698	CB CG	PRO PRO	215 215 ·	18.481	0.060	39.693	1.00 17.84	MTGL
ATOM	1699	C	PRO	215	18.728	2.576	41.395	1.00 17.33	MTGL
MOTA	1700	ŏ	PRO	215	17.847	3.078	42.092	1.00 17.47	MTGL
MOTA	1701	N	PHE	216	19.896	2.180	41.891	1.00 18.78	MTGL
MOTA	1702	CA	PHE	216	20.152	2.251	43,328	1.00 19.20	MTGL
ATOM	1703	CB	PHE	216	20.530	0.851	43.836	1.00 17.80	MTGL
ATOM	1704	CG	PHE	216	21.456	0.095	42.915	1.00 18.00	MTGL
MOTA	1705		PHE	216	22.673	0.641	42.522	1.00 18.05	MTGL
MOTA	1706	CD2	PHE	216	21.117	-1.172	42.456	1.00 17.34	MTGL
ATOM	1707	CEI	PHE	216	23.543	-0.064	41.680	1.00 17.92	MTGL
MOTA	1708	CE2	PHE	216	21.981	-1.887	41.614	1.00 17.55	MTGL
ATOM	1709	CZ	PHE	216	23.194	-1.331	41.228	1.00 16.80	MTGL
MOTA	1710	C	PHE	216	21.145	3.276	43.872	1.00 19.84	MTGL
ATOM	1711	0	PHE	216	21.726	3.068	44.940	1.00 21.57	MTGL
ATOM	1712	N	TYR	217	21.346	4.379	43.161	1.00 19.60	MTGL
MOTA	1713	CA	TYR	217	22.251	5.419	43.647	1.00 20.50	MTGL
MOTA	1714	CB	TYR	217	23.468	5.575	42.732	1.00 20.09	MTGL
ATOM	1715	CG	TYR	217	24.398	4.382	42.724	1.00 21.44	MTGL
ATOM	1716		TYR	217	24.956	3.895	43.909	1.00 21.17	MTGL
MOTA	1717		TYR	217	25.815	2.797	43.902	1.00 21.86	MTGL
MOTA	1718		TYR	217	24.721	3.739	41.529	1.00 20.83	MTGL.
ATOM	1719		TYR	217	25.577	2.642	41.511	1.00 21.46 1.00 21.33	MTGL MTGL
ATOM ATOM	1720 1721	CZ OH	TYR TYR	217 217	26.120 26.960	2.174 1.087	42.697 42.672	1.00 20.10	MTGL
ATOM	1722	C	TYR	217	21.520	6.752	43.727	1.00 20.10	MTGL
MOTA	1723	Ö	TYR	217	22.127	7.778	44.026		MTGL
ATOM	1724	N	SER	218	20.218	6.725	43.450	1.00 21.47	MTGL
ATOM	1725	CA	SER	218	19.387	7.926	43.475	1.00 22.44	MTGL
ATOM	1726	СВ	SER	218	20.043	9.050	42.677	1.00 23.02	MTGL
ATOM	1727	OG	SER	218	19.128	10.108	42.463	1.00 23.85	MTGL
MOTA	1728	С	SER	218	18.012	7.661	42.888	1.00 22.12	MTGL
ATOM	1729	0	SER	218	17.886	7.058	41.821	1.00 22.86	MTGL
MOTA	1730	N	SER	219	16.980	8.128	43.577	1.00 21.77	MTGL
ATOM	1731	CA	SER	219	15.615	7.938	43.111	1.00 22.44	MTGL
ATOM	1732	CB	SER	219	14.624	8.308	44.216	1.00 22.46	MTGL
ATOM	1733	OG	SER	219	14.793	9.658	44.607	1.00 22.44	MTGL
MOTA	1734	С	SER	219	15.333	8.782	41.867	1.00 22.56	MTGL
ATOM	1735	0	SER	219	14.282	8.646	41.247	1.00 23.34	MTGL
MOTA	1736	13	SER	220	16.267	9.653	41.503	1.00 22.13	MTGL
ATOM	1737	CA	SER	220	16.088	10.488	40.319	1.00 22.61	MTGL
ATOM	1738	CB	SER	220	17.037	11.691	40.358	1.00 23.25	MTGL
MOTA	1739	OG	SER	220	16.688	12.584	41.403	1.00 25.72	MTGL

Fig. 1 cont.

7 MOM	1740	^	~~~	000					
ATOM	1740	¢	SER	220	16.330	9.704	39.032	1.00 22.26	MTGL
ATOM	1741	0	SER	220	16.025	10.187	37.942	1.00 22.75	MTGL
ATOM	1742	N	ALA	221	16.872	8.495	39.160	1.00 20.89	MTGL
ATOM	1743	CA	ALA	221	17.164	7.667	37.996		
								1.00 20.44	MTGL
ATOM	1744	CB	ALA	221	18.266	6.644	38.343	1.00 19.75	MTGL
ATOM	1745	С	ALA	221	15.933	6.949	37.439	1.00 20.80	MTGL
MOTA	1746	0	ALA	221	15.941	5.731	37.265	1.00 20.53	MTGL
ATOM	1747	N	THR	222					
					14.875	7.705	37.163	1.00 20.53	MTGL
ATOM	1748	CA	THR	222	13.651	7.134	36.607	1.00 20.82	MTGL
MOTA	1749	CB	THR	222	12.464	8.120	36.690	1.00 20.95	MTGL
ATOM	1750	OGI	THR	222	12.792	9.310	35.966	1.00 21.38	MTGL
ATOM	1751		THR						
				222	12.152	8.483	38.137	1.00 21.55	MTGL
ATOM	1752	С	THR	222	13.848	6.809	35.129	1.00 20.30	MTGL
ATOM	1753	0	THR	222	14.754	7.334	34.479	1.00 20.05	MTGL
MOTA	1754	N	LEU	223	12.990	5.947	34.598	1.00 20.97	MTGL
ATOM	1755	CA	LEU	223	13.060				
						5.583	33.190	1.00 20.57	$\mathtt{MTGL}$
ATOM	1756	CB	LEU	223	12.116	4.412	32.894	1.00 21.05	$\mathtt{MTGL}$
MOTA	1757	CG	LEU	223	12.455	3.097	33.612	1.00 22,20	MTGL
ATOM	1758	CD1	LEU	223	11.415	2.039	33.276	1.00 22.93	MTGL
ATOM	1759		LEU	223	13.841	2.629			
ATOM							33.195	1.00 21.13	MTGL
	1760	C	LEU	223	12.674	6.800	32.346	1.00 20.76	MTGL
ATOM	1761	0	LEU	223	13.214	7.009	31.258	1.00 19.94	MTGL
MOTA	1762	N	SER	224	11.741	7.607	32.852	1.00 20.13	MTGL
ATOM	1763	CA	SER	224	11.311	8.804	32.128	1.00 20.71	
ATOM	1764	СВ	SER						MTGL
				224	10.096	9.448	32.812	1.00 21.29	MTGL
MOTA	1765	OG	SER	224	10.392	9.812	34.149	1.00 26.36	$\mathtt{MTGL}$
ATOM	1766	С	SER	224	12.452	9.815	32.036	1.00 18.99	MTGL
ATOM	1767	0	SER	224	12.641	10.450	30.999	1.00 19.23	MTGL
ATOM	1768	N	ALA	225	13.214	9.967	33.115		
ATOM	1769	CA						1.00 18.09	MTGL
			ALA	225	14.333	10.901	33.093	1.00 17.82	MTGL
MOTA	1770	CB	ALA	225	14.928	11.057	34.492	1.00 17.28	$\mathtt{MTGL}$
ATOM	1771	С	ALA	225	15.395	10.410	32.108	1.00 17.15	MTGL
ATOM	1772	0	ALA	225	16.018	11.208	31.410	1.00 18.25	MTGL
ATOM	1773	N	LEU	226	15.598	9.097	32.048		
ATOM	1774	CA						1.00 16.97	MTGL
	_		LEU	226	16.580	8.534	31.122	1.00 17.41	MTGL
ATOM	1775	ÇВ	LEU	226	16.693	7.017	31.303	1.00 17.39	MTGL
MOTA	1776	CG	LEU	226	17.711	6.325	30.389	1.00 17.54	MTGL
ATOM	1777	CD1	LEU	226	19.109	6.852	30.679	1.00 17.23	MTGL
ATOM	1778	CD2		226	17.658	4.824			
ATOM	1779	C					30.606	1.00 17.56	MTGL
	_		LEU	226	16.126	8.839	29.696	1.00 17.60	$\mathtt{MTGL}$
ATOM	1780	0	LEU	226	16.909	9.311	28.868	1.00 17.24	MTGL
MOTA	1781	И	LYS	227	14.854	8.566	29.423	1.00 17.18	MTGL
ATOM	1782	CA	LYS	227	14.277	8.811	28.105	1.00 18.16	MTGL
ATOM	1783	CB	LYS	227					
					12.780	8.488	28.120	1.00 18.24	MTGL
ATOM	1784	CG	LYS	227	12.007	8.984	26.890	1.00 18.81	$\mathtt{MTGL}$
ATOM	1785	CD	LYS	227	12.540	8.394	25.590	1.00 17.63	MTGL
ATOM	1786	ĊE	LYS	227	11.629	8.737	24.411	1.00 18.20	MTGL
ATOM	1787	NZ	LYS	227	12.191	8.269			
ATOM							23.111	1.00 17.92	MTGL
	1788		LYS	227	14.476	10.258	27.668	1.00 18.40	MTGL
MOTA	1789	0	LYS	227	14.978	10.526	26.576	1.00 18.56	MTGL
ATOM	1790	N	SER	228	14.078	11.190	28.529	1.00 18.71	MTGL
ATOM	1791	CA	SER	228	14.209	12.610	28.225		
ATOM	1792							1.00 18.63	MTGL
		CB	SER	228	13.584	13.449	29.344	1.00 19.90	MTGL
ATOM	1793	OG	SER	228	13.763	14.835	29.096	1.00 20.80	MTGL
MOTA	1794	С	SER	228	15.662	13.022	28.024	1.00 18.30	MTGL
ATOM	1795	0	SER	228	15.973	13.778	27.106	1.00 18.71	MTGL
ATOM	1796	N	SER	229	16.553				
ATOM						12.525	28.880	1.00 17.99	MTGL
ATOM	1797	CA	SER	229	17.969	12.862	28.768	1.00 18.28	MTGL

Fig. 1 cont.

									NAMOY
ATOM	1798	CB	SER	229	18.752	12.299	29.962	1.00 18.83	MTGL
ATOM	1799	OG	SER	229	20.127	12.641	29.867	1.00 17.92	MTGL
ATOM	1800	č	SER	229	18.577	12.339	27.463	1.00 18.05	MTGL
-				229	19.251	13.076	26.744	1.00 18.70	MTGL
ATOM	1801	0	SER					1.00 17.87	
ATOM	1802	N	LEU	230	18.338	11.070	27.149		
ATOM	1803	CA	LEU	230	18.884	10.503	25.920	1.00 17.26	MTGL
ATOM	1804	CB	LEU	230	18.620	8.994	25.860	1.00 16.24	MTGL
MOTA	1805	CG	LEU	230	19.265	8.162	26.976	1.00 16.12	MTGL
ATOM	1806	CD1		230	19.069	6.676	26.671	1.00 16.29	MTGL
		·CD2		230	20.749	8.473	27.084	1.00 12.97	MTGL
ATOM	1807							1.00 17.08	MTGL
ATOM	1808_	С	LEU	230	18.299	11.204	24.689		
ATOM	1809	0	LEU	230	19.014	11.458	23.721	1.00 15.52	MTGL
MOTA	1810	N	ASP	231	17.006	11.525	24.728	1.00 18.20	MTGL
ATOM	1811	CA	ASP	231	16.380	12.223	23.604	1.00 18.97	$\mathtt{MTGL}$
MOTA	1812	CB	ASP	231	14'.B96	12,494	23.878	1.00 20.35	MTGL
				231	13.985	11.337	23.455	1.00 20.69	MTGL
ATOM	1813	CG	ASP					1.00 21.48	MTGL
ATOM	1814	OD1		231	14.460	10.361	22.838		
MOTA	1815	ODS	ASP	231	12.775	11.418	23.738	1.00 20.71	MTGL
ATOM	1816	C	ASP	231	17.102	13.553	23.393	1.00 19.05	MTGL
MOTA	1817	0	ASP	231	17.423	13.927	22.265	1.00 20.05	MTGL
ATOM	1818	N	ASN	232	17.369	14.260	24.486	1.00 18.97	MTGL
ATOM	1819	CA	ASN	232	18.057	15.546	24.403	1.00 19.27	MTGL
	1820		ASN	232	18.126	16.219	25.781	1.00 19.34	MTGL
ATOM		CB				16.752	26.238	1.00 21.88	MTGL
MOTA	1821	CG	ASN	232	16.775				MTGL
MOTA	1822		ASN	232	15.911	17.054	25.420	1.00 23.78	
ATOM	1823	ND2		232	16.595	16.882	27.545	1.00 21.09	MTGL
MOTA	1824	C	ASN	232	19.459	15.397	23.834	1.00 19.42	MTGL
ATOM	1825	0	ASN	232	19.887	16.205	23.003	1.00 19.51	MTGL
ATOM	1826	N	MET	233	20.174	14.368	24.280	1.00 19.18	MTGL
MOTA	1827	CA	MET	233	21.533	14.124	23.803	1.00 19.15	MTGL
ATOM	1828	CB	MET	233	22.151	12.936	24.551	1.00 18.27	MTGL
ATOM	1829	CG	MET	233	22.433	13.191	26.029	1.00 19.33	MTGL
					22.806	11.662	26.940	1.00 19.17	MTGL
ATOM	1830	SD	MET	233				1.00 17.20	MTGL
ATOM	1831	CE	MET	233	24.330	11.165	26.125		MTGL
MOTA	1832	С	MET	233	21.510	13.833	22.305	1.00 19.80	
ATOM	1833	0	MET	233	22.356	14.314	21.547	1.00 19.41	MTGL
MOTA	1834	Ŋ	ALA	234	20.529	13.043	21.885	1.00 20.01	MTGL
ATOM	1835	CA	ALA	234	20.390	12.673	20.480	1.00 21.04	MTGL
ATOM	1836	CB	ALA	234	19.274	11.633	20.324	1.00 19.66	MTGL
ATOM	1837	C	ALA	234	20.111	13.879	19.583	1.00 21.48	
ATOM	1838	ŏ	ALA	234	20.761	14.055	18.549	1.00 20.87	
			LYS	235	19.156	14.715	19.985	1.00 22.48	
ATOM	1839	N				15.881	19.176	1.00 24.12	•
ATOM	1840	CA	LYS	235	18.804			1.00 26.52	
ATOM	1841	CB	LYS	235	17.507	16.515	19.681		
ATOM	1842	CG	LYS	235	17.053	17.695	18.835	1.00 33.00	
ATOM	1843	CD	LYS	235	15.744	18.274	19.331	1.00 36.39	
MOTA	1844	CE	LYS	235	15.288	19.436	18.451	1.00 40.33	
MOTA	1845	NZ	LYS	235	13.979	19.997	18.912	1.00 42.05	
ATOM	1846	C	LYS	235	19.900	16,937	19.145	1.00 22.78	MTGL
ATOM	1847	ŏ	LYS	235	20.041	17.660	18.169	1.00 21.57	
	1848		THR	236	20.688	17.014	20.209	1.00 23.01	
ATOM		N						1.00 22.42	MTGL
MOTA	1849	CA	THR	236	21.753	18.004	20.280		
ATOM	1850	CB	THR	236	22.146	18.289	21.744	1.00 22.63	
MOTA	1851		THR	236	20.973	18.616	22.495	1.00 23.14	
ATOM	1852	CG2	THR	236	23.118	19.459	21.818	1.00 22.49	
ATOM	1853	С	THR	236	23.020	17.635	19.506	1.00 22.72	
ATOM	1854	ŏ	THR	236	23.556	18.468	18.773	1.00 22.43	MTGL
ATOM	1855	N	TRP	237	23.495	16.398	19.655	1.00 21.45	
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Fig. 1 cont.

ATOM	1856	CA	TRP	237	24.728	15.984	18.984	1.00 21.17	MTGL
ATOM	1857	СВ	TRP	237	25.773	15.621	20.041	1.00 21.53	MTGL
ATOM	1858	CG	TRP	237	26,103	16.796	20.916	1.00 21.36	MTGL
							22.270	1.00 20.90	MTGL
ATOM	1859	CD2	TRP	237	25.684	17.004			
ATOM	1860	CE2	TRP	237	26.156	18.274	22.662	1.00 20.29	MTGL
ATOM	1861	CE3	TRP	237	24.957	16.237	23.191	1.00 20.64	MTGL
ATOM	1862	CD1	TRP	237	26.795	17.920	20.554	1.00 21.20	MTGL
ATOM	1863	NEI	TRP	237	26.827	18.811	21.595	1.00 19.36	MTGL
				237	25.919	18.799	23.935	1.00 20.39	MTGL
ATOM	1864	CZ2							
MOTA	1865		TRP	237	24.724	16.760	24.458	1.00 20.25	MTGL
MOTA	1866	CH2	TRP	. 237	25.205	18.028	24.817	1.00 20.45	MTGL
ATOM	1867	С	TRP	237	24.600	14.868	17.941	1.00 21.19	MTGL
ATOM	1868	0	TRP	237	25.561	14.555	17.238	1.00 20.33	MTGL
ATOM	1869	N	ASN	238	23.414	14.274	17.865	0.50 21.58	MTGL
	1870		ASN	238	23.119	13.212	16.908	0.50 21.97	MTGL
ATOM		CA							
MOTA	.1871	CB	ASN	238	22.847	13.829	15.534	0.50 23.20	MTGL
MOTA	1872	CG	ASN	238	21.696	14.822	15.560	0.50 24.82	MTGL
ATOM	1873	OD1	ASN	238	20.631	14.540	16.107	0.50 25.88	MTGL
MOTA	1874	ND2	ASN	238	21.904	15.989	14.960	0.50 26.50	MTGL
MOTA	1875	С	ASN	238	24.179	12.113	16.782	0.50 21.69	MTGL
ATOM	1876	ŏ	ASN	238	24.564	11.730	15.678	0.50 21.51	MTGL
				239	24.644	11.607	17.919	1.00 21.56	MTGL
ATOM	1877	N	LYS						
MOTA	1878	CA	LYS	239	25.639	10.534	17.938	1.00 20.81	MTGL
ATOM	1879	CB	PAR	239	26.732	10.832	18.971	1.00 21.93	MTGL
ATOM	1880	CG	LYS	239	27.684	11.957	18.598	1.00 21.60	MTGL
MOTA	1881	CD	LYS	239	28.521	11.569	17.396	1.00 23.06	MTGL
ATOM	1882	CE	LYS	239	29.543	12.633	17.053	1.00 23.30	MTGL
ATOM	1883	NZ	LYS	239	30.266	12.280	15.800	1,00 22.03	MTGL
MOTA	1884	С	LYS.	239	24.927	9.243	18.331	1.00 20.23	MTGL
ATOM	1885	Õ	LYS	239	23.814	9.287	18.856	1.00 19.43	MTGL
ATOM	1886	N	GLU	240	25.548	8.096	18.072	1.00 19.70	MTGL
MOTA	1887		GLU	240	24.933	6.835	18.467	1.00 19.84	MTGL
		CA						1.00 21.53	MTGL
ATOM	1888	CB	GLU	240	25.702	5.633	17.912		
ATOM	1889	CG	GLU	240	25.612	5.485	16.402	1.00 24.54	MTGL
MOTA	1890	CD	GĽŰ	240	25.950	4.081	15.930	1.00 26.26	MTGL
ATOM	1891	OE1	GLU	240	26.984	3.532	16.366	1.00 27.61	MTGL
ATOM	1892	OE2	GLU	240	25.179	3.527	15.118	1.00 28.35	MTGL
ATOM	1893	С	GLU	240	24.972	6.823	19.985	1.00 18.12	MTGL
ATOM	1894	ō	GLU.		25.945	7.269	20.589	1.00 16.94	MTGL
ATOM	1895	Ŋ	ILE	241	23.910	6.320	20.598	1.00 17.17	MTGL
								1.00 17.75	MTGL
ATOM	1896	CA	ILE	241	23.816	6.290	22.049		
ATOM	1897	CB	ILE	241	22.639	7.161	22.509	1.00 18.47	MTGL
ATOM	1898		ILE	241	22.411	6.997	24.013	1.00 19.08	MTGL
ATOM	1899	CG1	ILE	241	22.918	8.617	22.126	1.00 17.74	MTGL
ATOM	1900	CD1	ILE	241	21.732	9.539	22.297	1.00 18.08	MTGL
MOTA	1901	С	ILE	241	23.651	4.894	22.625	1.00 17.68	MTGL
ATOM	1902	0	ILE	241	23.020	4.026	22.015	1.00 16.98	MTGL
ATOM	1903	N	ALA	242	24.219	4.683	23.809	1.00 17.80	MTGL
					24.115	3.389	24.465	1.00 17.48	MTGL
ATOM	1904	CA	ALA	242					
ATOM	1905	CB	ALA	242	25,170	2.433	23.906	1.00 16.79	MTGL
ATOM	1906	C	ALA	242	24.244	3.457	25.977	1.00 16.97	MTGL
MOTA	1907	0	ALA	242	24.966	4.291	26.520	1.00 16.47	MTGL
ATOM	1908	N	VAL	243	23.505	2.586	26.654	1.00 16.88	MTGL
ATOM	1909	CA	VAL	243	23.594	2.478	28.098	1.00 16.35	MTGL
MOTA	1910	CB	VAL	243	22.261	2.003	28.715	1.00 15.54	MTGL
ATOM	1911		VAL	243	22.470	1.580	30.159	1.00 16.43	MTGL
ATOM	1912		VAL	243	21,238	3.133	28.655	1.00 15.23	MTGL
MOTA	1913	C	VAL	243	24.667	1.396	28.212	1.00 16.01	MTGL
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Fig. 1 cont.

		_							
ATOM	1914	0	VAL	243	24.424	0.243	27.856	1.00 16.07	MTGL
MOTA	1915	N	VAL	244	25.860	1.774	28.665	1.00 15.48	MTGL
ATOM	1916	CA		244		0.822	28.758	1.00 15,55	
			VAL		26.971				MTGL
MOTA	1917	CB	VAL	244	28.292	1.501	28.345	1.00 15.25	MTGL
ATOM	1918	CG1	VAL	244	28.167	2.024	26.922	1.00 15.71	MTGL
MOTA	1919		VAL	244	28.618	2.646	29.294	1.00 14.98	MTGL
	-								
ATOM	1920	C	VAL	244	27.163	0.125	30.097	1.00 15.27	MTGL
MOTA	1921	0	VAL	244	28.052	-0.710	30.244	1.00 16.53	MTGL
ATOM	1922	N	GLU	245	26.326	0.464	31.068	1.00 15.31	MTGL
MOTA	1923	CA	GLU	245	26.387	-0.145	32.391	1.00 15.54	MTGL
ATOM	1924	CB	GLU	245	27.390	0.581	33.301	1.00 15.71	MTGL
MOTA	1925	CG	GLU	245	28.833	0.193	33.105	1.00 17.89	MTGL
ATOM	1926	CD	GLU		29.738				
				245		0.777	34.177	1.00 19.37	MTGL
ATOM	1927	OE1	GLU	245	29.322	0.824	35.359	1.00 18.55	MTGL
ATOM	1928	OE2	GLU	245	30.867	1.174	33.827	1.00 20.37	MTGL
ATOM	1929	C	GLU	245	25.024	-0.053	33.043	1.00 15.41	MTGL
			-						
MOTA	1930	0	GLU	245	24.421	1.014	33.060	1.00 16.55	MTGL
ATOM	1931	N	THR	246	24.533	-1.174	33.563	1.00 15.11	MTGL
ATOM	1932	CA	THR	246	23.266	-1.185	34.280	1.00 14.75	MTGL
MOTA	1933	CB	THR	246	22.053	-1.052	33.322	1.00 15.60	MTGL
ATOM	1934	OG1	THR	246	20.884	-0.721	34.085	1.00 14.95	MTGL
ATOM	1935	CG2	THR	246	21.809	-2.352	32.564	1.00 14,91	MTGL
ATOM	1936		THR	246	23,168				
		Ç				-2.467	35.100	1.00 14.67	MTGL
ATOM	1937	0	THR	246	23.853	-3.451	34.807	1.00 15.70	MTGL
ATOM	1938	N	ASN	247	22.331	-2.441	36.134	1.00 14.38	MTGL
ATOM	1939	CA	ASN	247	22.128	-3.579	37.035	1.00 14.91	MTGL
MOTA	1940	CB	ASN	247	23.012	-3.462	38.294	1.00 15.25	MTGL
MOTA	1941	CG	ASN	247	24.397	-4.085	38.150	1.00 16.92	MTGL
ATOM	1942	OD1	ASN	247	25.212	-3.972	39.068	1.00 16.53	MTGL
ATOM	1943	ND2		247		-4.746			MTGL
					24.668			1.00 14.82	
MOTA	1944	С	ASN	247	20.693	-3.554	37.560	1.00 15.99	MTGL
MOTA	1945	0	ASN	247	20.057	-2.496	37.609	1.00 15.64	MTGL
MOTA	1946	N	TRP	248	20.194	-4.723	37.946	1.00 15.53	MTGL
	1947								
ATOM		CA	TRP	248	18.893	-4.830	38.600	1.00 16.36	MTGL
MOTA	1948	CB	TRP	248	17.732	-5.127	37.657	1.00 14.84	$\mathtt{MTGL}$
ATOM	1949	CG	TRP	248	16,455	~5.135	38.445	1.00 13.73	MTGL
MOTA	1950		TRP	248	15.743	-3.989	38.940	1.00 14.11	
									MTGL
ATOM	1951	CEZ	TRP	248	14.684	-4.467	39.739	1.00 12.13	MTGL
MOTA	1952	CE3	TRP	248	15.902	-2.603	38.786	1.00 14.57	MTGL
ATOM	1953	CD1	TRP	248	15.812	-6.224	38.949	1.00 13.26	MTGL
ATOM	1954								
		NEI		248	14.751	-5.833	39.728	1.00 13.69	MTGL
ATOM	1955	CZ2	TRP	248	13.784	-3.613	40.384	1.00 14.00	MTGL
ATOM	1956	CZ3	TRP	248	15.008	-1.751	39.427	1.00 13.98	MTGL
ATOM	1957		TRP	248	13.962	-2.260	40.218	1.00 14.50	MTGL
MOTA	1958	C	TRP	248	19.080	-5.972	39.576	1.00 16.41	MTGL
MOTA	1959	0	TRP	248	19.507	-7.060	39.200	1.00 17.70	MTGL
ATOM	1960	N	PRO	249	18.765	-5.739	40.850	1.00 17.62	MTGL
ATOM	1961	CD	PRO	249	18.316	-4.468	41.449	1.00 17.41	MTGL
ATOM	1962	CA	PRO	249	18.933	-6.774	41.868	1.00 17.81	MTGL
ATOM	1963	CB	PRO	249	19.010	-5.961	43.156	1.00 18.08	MTGL
ATOM	1964	CG	PRO	249	18.056	-4.857	42.892	1.00 20.03	
									MTGL
MOTA	1965	C	PRO	249	17.922	-7.898	41.972	1.00 18.16	MTGL
ATOM	1966	0	PRO	249	16.729	-7.722	41.728	1.00 18.74	MTGL
ATOM	1967	N	ILE	250	18.426	-9.074	42.322	1.00 18.86	MTGL
ATOM	1968	CA	ILE	250	17.561		42.549	1.00 20.06	MTGL
ATOM	1969	CB	ILE	250	18.189	-11.544	42.040	1.00 20.52	MTGL
ATOM	1970	CG2	ILE	250	18.230		40.518	1.00 19.08	MTGL
ATOM	1971	CG1		250	19.590		42.614	1.00 20.81	
LI LOG	T 2 1 T	~67	بتاديد	230	TA.2A0	-11./34	44.014	1.00 20.81	MTGL

Fig. 1 cont.

ATOM	1972	CD1	ILE	250	20.222 -	-13.061	42.216	1.00 21.09	MTGL
ATOM	1973		ILE	250	17.408 -		44.075	1.00 19.97	MTGL
ATOM	1974	Ō	ILE	250	16.659 -	-11.028	44.637	1.00 20.48	MTGL
ATOM	1975	N	SER	251	18.127	-9.327	44.735	1.00 20.21	MTGL
ATOM	1976	CA	SER	251	18.072	-9.206	46.188	1.00 21.30	MTGL
ATOM	1977	CB	SER	251	18.878 -		46.843	1.00 22.63	MTGL
ATOM	1978	OG	SER	251	18,757 -	-10.273	48.253	1.00 24.04	MTGL
ATOM	1979	С	SER	251	18.603	-7.855	46.658	1.00 21.50	MTGL
ATOM	1980	0	SER	251	19.735	-7.485	46.343	1.00 21.25	MTGL
MOTA	1981	N	CYS	252	17.784	-7.112	47.400	1.00 21.87	MTGL
MOTA	1982	CA	CYS	252	18.194	-5.806	47.918	1.00 23.27	MTGL
MOTA	1983	C .	CYS	252	17.529	<b>~</b> 5.505	49.263	1.00 24.17	MTGL
MOTA	1984	0	CYS	252	16.654	-4.647	49.340	1.00 24.61	MTGL
MOTA	1985	CB	CYS	252	17.840	-4.684	46.927	1.00 23.57	MTGL
MOTA	1986	SG	CYS	252	18.756	-3.154	47.311	1.00 23.83	MTGL
MOTA	1987	N	PRO	253	17.951	-6.199	50.340	1.00 25.34	MTGL
MOTA	1988	CD	PRO	253	18.950	-7.281	50.290	1.00 26.08	MTGL
MOTA	1989	CA	PRO	253	17.428	-6.052	51.707	1.00 25.93	MTGL
ATOM	1990	CB	PRO	253	18.308	-7.001	52.518	1.00 26.63	MTGL
MOTA	1991	CG	PRO	253	18.627	-8.068	51.539	1.00 27.12	MTGL
ATOM	1992	С	PRO	253	17.416	-4.645	52.294	1.00 26.16	MTGL
ATOM	1993	0	PRO	253	16.415	-4.223	52.865	1.00 26.46	MTGL
MOTA	1994	N	ASN	254	18.526	-3.922	52.178	1.00 26.96	MTGL
ATOM	1995	CA	ASN	254	18.574	-2.560	52.713	1.00 27.76	MTGL
MOTA	1996	CB	ASN	254	19.145	-2.538	54.137	1.00 29.54	MTGL
ATOM	1997	CG	ASN	254	20.541	-3.097	54.220	1.00 31.33	MTGL
ATOM	1998	OD1		254	20.854	-4.102	53.587	1.00 34.28	MTGL MTGL
ATOM	1999	ND2		254	21.388	-2.465	55.028	1.00 30.87	MTGL .
ATOM	2000	С	ASN	254	19.329	-1.580	51,834	1.00 26.98	MTGL
ATOM	2001	0	ASN	254	20.525	-1.355	51.990	1.00 26.72	MTGL
MOTA	2002	N	PRO	255	18.623	-0.993	50.873	1.00 26.12 1.00 25.65	MTGL
MOTA	2003	CD	PRO	255	17.274	-1.385	50.443	1.00 25.85	MTGL
ATOM	2004	CA	PRO	255	19.222	-0.023	49.957 48.913	1.00 25.50	MTGL
ATOM	2005	CB	PRO	255	18.128	0.211	49,550	1.00 25.88	MTGL
MOTA	2006	CG	PRO	255	16,895	-0.262 1.279	50.637	1.00 25.08	MTGL
MOTA	2007	C	PRO	255	19.638 18.993	1.735	51.586	1.00 24.66	MTGL
ATOM	2008	Ο.	PRO	255	20,717	1.755	50.128	1.00 23.54	MTGL
ATOM	2009	N	ARG	256 256	21.219	3.131		1.00 24.56	MTGL
ATOM	2010 2011	CA CB	ARG	256	22.679	3.345	50.230	1.00 26.20	MTGL
ATOM ATOM	2011	CG	ARG	256	23.290	4.673	50.685	1.00 29.88	MTGL
ATOM	2013	CD	ARG	256	23.244	4.843	52.205	1.00 33.75	MTGL
ATOM	2013	NE	ARG	256	24.112	3.900	.52.913	1.00 36.98	MTGL
ATOM	2015	CZ	ARG	256	24.215	3.826	54.241	1.00 38.13	MTGL
ATOM	2016		ARG	256	23.503	4.638	55.016	1.00 37.96	MTGL
ATOM	2017		ARG	256	25.034	2.942	54.796	1.00 38.27	MTGL
ATOM	2018	C	ARG	256	20.346	4.291	50.152	1.00 24.09	MTGL
ATOM	2019	ō	ARG	256	20.223	5.312	50.820	1.00 22.82	MTGL
MOTA	2020	N	TYR	257	19.740	4.129	48.978	1.00 23.76	MTGL
ATOM	2021	CA	TYR	257	18.869	5.162	48.417	1.00 24.47	MTGL
MOTA	2022	CB	TYR	257	19.506	5.829	47.197	1.00 25.66	MTGL
ATOM	2023	CG	TYR	257	20.889	6.365	47.430	1.00 27.18	MTGL
ATOM	2024		TYR	257	22.003	5.538	47.316	1.00 27.30	MTGL
ATOM	2025		TYR	257	23.283	6.020	47.567	1.00 28.24	MTGL
ATOM	2026	CD2		257	21.086	7.693	47.802	1.00 28.37	MTGL
ATOM	2027		TYR	257	22,363	8.184	48.058	1.00 28.50	MTGL
ATOM	2028	CZ	TYR	257	23.455	7.341	47.940	1.00 29.46	MTGL
ATOM	2029	ОН	TYR	257	24.720	7.814	48.215	1.00 30.61	MTGL

Fig. 1 cont.

		_	mvn	257	17:539	4.578	47.986	1.00 24.30	MTGL
MOTA	2030	_	TYR	257 257	17.450	3.408	47.619	1.00 24.04	MTGL
ATOM	2031	_	TYR	257 258	16.507	5.411	48.018	1.00 24.57	MTGL
ATOM	2032		SER	258	15.178	4.984	47.607	1.00 24.95	MTGL
MOTA	2033		SER		14,162	6.084	47.930	1.00 25.55	MTGL
ATOM	2034		SER	258	14.162	6.471	49.292	1.00 27.69	MTGL
MOTA	2035		SER	258	15.230	4.746	46.102	1.00 23.31	MTGL
MOTA	2036		SER	258	15.949	5,449	45.392	1.00 23,48	MTGL
ATOM	2037		SER	258		3.754	45.619	1.00 22.69	MTGL
MOTA	2038		PHE	259	14.488	3.452	44.190	1.00 23.46	MTGL
ATOM	2039		PHE	259	14.459 13.961	2.022	43.958	1.00 22.78	MTGL
ATOM	2040		PHE	259		0.990	43.984	1.00 22.99	MTGL
MOTA	2041	CG	PKE	259	15.051	0.904	45.066	1.00 24.03	MTGL
MOTA	2042	CD1		259	15.923	0.112	42.919	1.00 22.03	MTGL
MOTA	2043	CD2		259	15.218	-0.046	45.089	1.00 24.16	MTGL
MOTA	2044	CEl		259	16.945	-0.839	42.929	1.00 22.81	MTGL
MOTA	2045	CE2		259	16.233	-0.918	44.019	1.00 23.26	MTGL
MOTA	2046	CZ	PHE	259	17.103	4.429	43.411	1.00 23.33	MTGL
MOTA	2047	C	PHE	259	13.580	5.048	43.975	1.00 23.29	MTGL
MOTA	2048	0	PHE	259	12.681	4.581	42.100	1.00 23.87	MTGL
ATOM	2049	N	PRO	260	13.840		41.338	1.00 23.34	MTGL
MOTA	2050	CD	PRO	260	14.959	4.002 5.492	41.259	1.00 23.83	MTGL
ATOM	2051	CA	PRO	260	13.057	5.346	39.888	1.00 23.96	MTGL
ATOM	2052	CB	PRO	260	13.711	5.012	40.229	1.00 23.75	MTGL
MOTA	2053	CG	PRO	260	15.138	5.062	41.255	1.00 24.68	MTGL
MOTA	2054	C	PRO	260	11.594	3.867	41.233	1.00 22.71	MTGL
MOTA	2055	0	PRO	260	11.287	6.042	41.274	1.00 24.81	MTGL
ATOM	2056	N	SER	261	10.700 9.267	5,783	41.298	1.00 25.73	MTGL
MOTA	2057	CA	SER	261	8.494	7.107	41.254	1.00 26.69	MTGL
ATOM	2058	CB	SER	261	8,667	7.757	40.003	1.00 27.65	MTGL
MOTA	2059	ÒG	SER	261	8.725	4.862	40.207	1.00 25.31	MTGL
ATOM	2060	c	SER	261	7,853	4.048	40.488	1.00 25.28	MTGL
MOTA	2061	0	SER	261	9.214	4.979	38.973	1.00 26.49	MTGL
MOTA	2062	N	ASP	262	8.678	4.131	37.909	1.00 27.78	MTGL
ATOM	2063	CA	ASP	262	8.762	4.824	36.535	1.00 27.44	MTGL
MOTA	2064	CB	ASP	262	10.166	5.267	36.170	1.00 29.75	MTGL
ATOM	2065	CG	ASP	262	11.138	4.673	36.681	1.00 29.62	MTGL
ATOM	2066		ASP	262	10.289	6.207	35.349	1.00 29.82	MTGL
ATOM	2067		ASP	262 · 262	9.259		37.816	1.00 28.89	MTGL
ATOM	2068	C	ASP	262	9.063	2.037	36.812	1.00 29.03	$\mathtt{MTGL}$
MOTA	2069	0.	ASP	263	9.968	2.291	38.857	1.00 29.21	MTGL
ATOM	2070	N	VAL	263	10.529	0.941	38.878	1.00 29.98	$\mathtt{MTGL}$
MOTA	2071	CA	VAL VAL	263	12.063	0.930	38.613	1.00 29.51	MTGL
ATOM	2072	CB		263	12.355	1.468	37.226	1.00 28.86	MTGL
ATOM	2073		VAL	263	12.788	1.751	39.669	1.00 29.09	MTGL
ATOM	2074		VAL VAL	263	10.254	0.257	40.218	1.00 30.76	MTGL
ATOM	2075	C		263	10.672	-0.879		1.00 30.49	MTGL
MOTA	2076	0	VAL	264	9.534	0.941	41.108	1.00 31.82	MTGL
ATOM	2077	N	LYS		9.215	0.394		_	MTGL
ATOM	2078	CA	LYS	264 264	8.570	1.464	43.317	1.00 34.40	MTGL
ATOM	2079	CB	LYS		9,566				MTGL
ATOM	2080	CG	LYS	264 264	8,859				MTGL
ATOM	2081	CD	LYS		9.844				MTGL
ATOM	2082	CE	LYS LYS		9.148				MTGL
MOTA	2083		LYS		8.321		_		MTGL
MOTA	2084	C	LYS		8.267				MTGL
ATOM	2085		ASN		7.612				MTGL
ATOM	2086		ASN		6.738				MTGL
MOTA	2087	CM	いりい	<u> </u>	0,750				

Fig. 1 cont.

n mon	2088	CD	ASN	265	5.587	-1.898	40.236	1.00 34.35	MTGL
ATOM		CB	ASN	265	6.074	-1.544	38.845	1.00 36.81	MTGL
ATOM	2089			265	6.837	-0.593	38.667	1.00 37.33	MTGL
MOTA	2090	001			5.638	-2.311	37.848	1.00 38.71	MTGL
ATOM	2091	ND2		265	7.504	-3.436	40.689	1.00 30.70	MTGL
MOTA	2092	С	ASN	265		-4.555	40.744	1.00 30.83	MTGL
ATOM	2093	0	ASN	265	6.998		40.744	1.00 28.28	MTGL
ATOM	2094	N	ILE	266	8.719	-3.226		1.00 25.48	MTGL
MOTA	2095	ÇA	ILE	266	9.517	-4.336	39.687		MTGL
MOTA	2096	CB	ILE	266	10.651	-3.848	38.767	1.00 23.96	
ATOM	2097	CG2	ILE	266	11.449	-5.046	38.257	1.00 23.40	MTGL
ATOM.	2098	CG1	ILE	266	10.067	-3.054	37.594	1.00 23.38	MTGL
ATOM	2099	CD1	ILE	266	11.114	-2.516	36.627	1.00 22.30	MTGL
ATOM	2100	C	ILE	266	10.122	-5.094	40.867	1.00 24.88	MTGL
MOTA	2101	Õ	ILE	266	10.825	-4.520	41.691	1.00 22.68	MTGL
ATOM	2102	N	PRO	267	9.850	-6.404	40.960	1.00 24.25	MTGL
ATOM	2102	CD	PRO	267	9,012	-7.212	40.051	1.00 23.79	MTGL
			PRO	267	10.374	-7.225	42.052	1.00 23.72	MTGL
MOTA	2104	CA		267	9.542	-8.497	41.946	1.00 24.48	MTGL
ATOM	2105	CB	PRO		9.373	-8.633	40.455	1.00 24.22	MTGL
ATOM	2106	CG	PRO	267	11.865	-7.526	41.943	1.00 23.20	MTGL
ATOM	2107	С	PRO	267			40.851	1.00 22.29	MTGL
MOTA	2108	0	PRO	267	12.437	-7.515	43.090	1.00 22.29	MTGL
ATOM	2109	N	PHE.		12.487	-7.781		1.00 22.67	MTGL
MOTA	2110	CA	PHE	268	13.898	-8.134	43.119		MTGL
ATOM	2111	CB	PHE	268	14.533	-7.757	44.462	1.00 22.68	MTGL
ATOM	2112	CG	PHE	268	14.493	-6.285	44.754	1.00 22.93	
ATOM	2113	CD1	PHE	268	14.838	~5.360	43.773	1.00 22.68	MTGL
ATOM	2114	CD2	PHE	268	14.115	-5.821	46.008	1.00 23.18	MTGL
ATOM	2115		PHE	268	14.806	-3.993	44.037	1.00 23.40	MTGL
ATOM	2116	CE2	PHE	268	14.079	-4.454	46.283	1.00 23.36	MTGL
ATOM	2117	CZ	PHE	268	14.425	-3.539	45.298	1.00 23.35	MTGL
ATOM	2118	C	PHE	268	13,925	-9.643	42.921	1.00 21.88	MTGL
MOTA	2119	ŏ	PHE	268	13.780	-10.414	43.873	1.00 21.02	MTGL
ATOM	2120	N	SER	269		-10.049	41.667	1.00 21.08	$\mathtt{MTGL}$
MOTA	2121	CA	SER	269		-11.457	41.294	1.00 20.72	$\mathtt{MTGL}$
	2122	CB	SER	269		-12.052	41.417	1.00 19.79	MTGL
MOTA	2123	OG	SER	269		-11.416	40.509	1.00 19.06	MTGL
MOTA		C	SER	269		-11.546	39.844	1.00 20.32	MTGL
ATOM	2124					-10.530	39,161	1.00 19.97	MTGL
ATOM	2125	<u>.</u> .	SER	269		-12.767	39.354	1.00 21.15	MTGL
ATOM	2126	N	PRO	270			40.075	1.00 20.43	MTGL
MOTA	2127	CD	PRO	270		-14.054	37.958	1.00 20.91	MTGL
ATOM	2128	CA	PRO	270		-12.915		1.00 20.78	MTGL
ATOM	2129	CB	PRO	270		-14.426	37.809	1.00 20.58	MTGL
MOTA	2130	CG	PRO	270		-14.852	39.196	1.00 20.33	MTGL
MOTA	2131	С	PRO	270	14.169	-12.348	37.016		MTGL
MOTA	2132	0	PRO	270		-11.688	36.028	1.00 20.64	
ATOM	2133	N	GLU	271		-12.605		1.00 21.15	MTGL
ATOM	2134	CA	GLU	271	11.797	-12.102	36.508	1.00 21.55	MTGL
ATOM	2135	CB	GLU	271	10.446	-12.538	37.082	1.00 22.38	MTGL
ATOM	2136	CG	GLU	271		-14.036	37.003	1.00 25.49	MTGL
ATOM	2137	CD	GLU	271	11.082	-14.873	37.870	1.00 26.37	MTGL
ATOM	2138		ı GLU		11.447	-14.415	38.970	1.00 26.39	MTGL
MOTA	2139		2 GLU			-15.997		1.00 27.82	MTGL
ATOM	2140	C C	GLU	271		-10.577			MTGL
		õ	GLU		11.640			1.00 20.80	MTGL
MOTA	2141				12.166	-9.993		1.00 19.71	MTGL
ATOM	2142		GLY						MTGL
ATOM	2143	CA	GLY		12.271				MTGL
ATOM	2144		GLY		13.415				MTGL
ATOM	2145	0	GLY	272	13.284	-0.941	50.205	1.00 17.12	

Fig. 1 cont.

	22.46		CT N	273	14.534	-8.734	36.859	1.00 17.61	MTGL
ATOM	2146 2147		GLN GLN	273		-8.299	36.074	1.00 18.43	MTGL
ATOM.	2148		GLN	273		-9.260	36.230	1.00 17.76	MTGL
ATOM	2149	CG	GLN	273		-9.345	37.610	1.00 19.26	MTGL
MOTA	2150		GLN	273	18.720 -		37.607	1.00 19.87	MTGL
MOTA	2150	OE1		273	18.726 -	11.304	37.073	1.00 18.60	MTGL
MOTA	2152	NE2		273	19.793	-9.667	38.198	1.00 19.12	MTGL
MOTA	2152	C	GLN	273	15.300	-8.270	34.607	1.00 18.09	MTGL
ATOM	2154	0	GLN ·			-7.353	33.869	1.00 17.98	MTGL
ATOM	2155	N	THR	274	14.579	-9.305	34.193	1.00 17.84	MTGL
ATOM	2156	CA	THR	274	14.131	-9.433	32.815	1.00 17.91	MTGL
MOTA	2157	CB	THR	274	13.293 -		32.637	1.00 18.13	MTGL
ATOM	2158	OG1	THR	274	14.128 -	-11.857	32.859	1.00 19.81	MTGL
ATOM	2159	CG2		274	12.695 -	-10.777	31.231	1.00 19.04	MTGL
ATOM	2160	C	THR	274	13.293	-8.219	32.428	1.00 17.34	MTGL
ATOM	2161	ŏ	THR	274	13.504	-7.619	31.376	1.00 16.72	MTGL
MOTA	2162	N	THR	275	12.351	-7.859	33.294	1.00 16.98	MTGL
ATOM	2163	CA	THR	275	11.483	-6.712	33.056	1.00 17.24	MTGL
ATOM	2164	CB	THR	275	10.425	-6.574	34.169	1.00 17.29	MTGL
ATOM	2165		THR	275	9.587	-7.735	34.181	1.00 17.49	. MTGL
ATOM	2166		THR	275	9.563	-5.331	33.937	1.00 16.88	MTGL
ATOM	2167	C	THR	275	12.270	-5.405	32.982	1.00 17.05	MTGL
ATOM	2168	õ	THR	275	12.090	-4.618	32.052	1.00 17.86	MTGL
MOTA	2169	N	PHE	276	13.139	-5.174	33.963	1.00 16.71	MTGL
ATOM	2170	CA	PHE	276	13.937	-3.949	34.000	1.00 15.62	MTGL
ATOM	2171	CB	PHE	276	14.781	-3.890	35.278	1.00 15.45	MTGL
ATOM	2172	CG	PHE	276	15.621	-2,646	35.389	1.00 16.62	MTGL
ATOM	2173		PHE	276	15.048	-1.437	35.7 <b>77</b>	1.00 17.56	MTGL
ATOM	2174	CD2	PHE	276	16.976	-2.675	35.077	1.00 17.00	MTGL
ATOM	2175		PHE	276	15.817	-0.272	35.860	1.00 18.40	MTGL
MOTA	2176	CE2	PHE	276	17.757	-1.518	35.155	1.00 18.28	MTGL
ATOM	2177	CZ	PHE	276	17.176	-0.314	35.546	1.00 17.73	MTGL
MOTA	2178	C	PHE	276	14.866	-3.825	32.796	1.00 16.42	MTGL MTGL
ATOM	2179	0	PHE	276	14.907	-2.785	32.136	1.00 17.18	MTGL
ATOM	2180	N	ILE	277	15.627	-4.881	32.520	1.00 15.71 1.00 14.72	MTGL
MOTA	2181	CA	ITE	277	16.558	-4.864	31.399	1.00 14.72	MTGL
ATOM	2182	CB	ILE	277	17.364	-6.181	31.330	1.00 14.70	MTGL
MOTA	2183		ILE	277	18.227	-6.209	30.063	1.00 14.86	MTGL
ATOM	2184		ILE	277	18.238	-6.305	32.587 32.727	1.00 14.36	MTGL
ATOM	2185		ILE	277	18.945	-7.635	30.081	1.00 14.58	MTGL
ATOM	2186	C	ILE	277	15.832	-4.643 -3.868	29.250	1.00 14.01	MTGL
ATOM	2187	0	ILE	277	16.286	-5.330	29.890	1.00 14.56	MTGL
MOTA	2188	N	THR	278	14.708	-5.182	28.663	1.00 15.56	MTGL
ATOM	2189	CA	THR	278	13.930 12.724	-6.159	28.635	1.00 15.82	MTGL
ATOM	2190	CB	THR	278	13.203	-7.505	28.742	1.00 16.63	MTGL
ATOM	2191	OG1		278	11.942	-6.017	27.329	1.00 15.47	MTGL
MOTA	2192		THR	278 2 <b>7</b> 8	13.411	-3.747	28.530	1.00 15.31	MTGL
MOTA	2193	C	THR		13.435	-3.168	27.446	1.00 16.65	MTGL
ATOM	2194	0	THR	278 279	12.946	-3.174	29.634	1,00 15.85	MTGL
MOTA	2195	N	ASN		12.430	-1.808	29.609	1.00 16.36	MTGL
ATOM	2196 2197	CA CB	ASN ASN		11.743	-1.475	30.939	1.00 15.56	MTGL
ATOM	2197	CG	ASN	_	10.388	-2.159	31.077	1.00 17.29	MTGL
ATOM	2198		ASN L ASN		9.939	-2.848	30.167	1.00 15.98	t MTGL
MOTA MOTA	2200		2 ASN		9.736	-1.966		1.00 17.61	MTGL
ATOM	2201	Ć	ASN		13.520	-0.783		1.00 16.68	MTGL
ATOM	2202	õ	ASN		13.300	0.155		1.00 16.98	MTGL
ATOM	2203	N	VAL		14.695	-0.950		1.00 16.27	MTGL
AJOH	-203								

Fig. 1 cont.

			****	280	15.782	-0.013	29.641	1.00 15.63	MTGL
MOTA			VAL	_	17.005	-0.283	30.545	1.00 15.75	MTGL
ATOM			VAL	280	18.171	0.623	30.126	1.00 14.59	MTGL
ATOM		CG1		280		~0.023	32.007	1.00 14.29	MTGL
MOTA		CG2		280	16.634	-0.144	28.183	1.00 15.42	MTGL
ATOM	2208	C	VAL	280	16.203		27.512	1.00 14.80	MTGL
ATOM	2209	0	VAL	280	16.483	0.852	27.512	1.00 14.47	MTGL
ATOM	2210	N	ALA	281	16.236	-1.381	26.315	1.00 15.95	MTGL
ATOM	2211	CA	ALA	281	16.614	-1.645		1.00 15.85	MTGL
MOTA	2212	CB	ALA	281	16.573	-3.147	26.035	1.00 16.21	MTGL
ATOM	2213	С	ALA	281	15.662	-0.922	25.369	1.00 15.33	MTGL
ATOM	2214	0	ALA	281	16.087	-0.290	24.403	1.00 16.95	MTGL
MOTA	2215	N	ASN	282	14.369	-1.018	25.653	1.00 17.84	MTGL
MOTA	2216	CA	ASN	282	13.383	-0.386	24.792	1.00 17.04	MTGL
ATOM	2217	CB	ASN	282	12.015	-1.013	25.021	1.00 19.13	MTGL .
ATOM	2218	CG	ASN	282	11.924	-2.398	24.400	1.00 20.19	MTGL
ATOM	2219	OD1	ASN	282	12.393	-2.605	23.289		MTGL
ATOM	2220	ND2	ASN	282	11.328	-3.341	25.108	1.00 19.74	MTGL
ATOM	2221	С	ASN	282	13.337	1.124	24.910	1.00 18.52	MTGL
ATOM	2222	0	ASN	282	12.841	1.806	24.011	1.00 17.57	MTGL
MOTA	2223	И	ILE	283	13.851	1.651	26.015	1.00 18.29	MTGL
ATOM	2224	CA	ILE	283	13.902	3.095	26.168	1.00 18.86	MTGL
ATOM	2225	CB	ILE	283	14.254	3.496	27.603	1.00 19.57	MTGL
ATOM	2226	CG2	ILE	283	14.818	4.917	27.636	1.00 20.74	MTGL
ATOM	2227		ILE	283	13.003	3.365	28.471	1.00 21.83	
ATOM	2228	CD1	ILE	283	13.214	3.728	29.909	1.00 25.75	MTGL
ATOM	2229	С	ILE	283	14.994	3.566	25.209	1.00 17.96	MTGL
ATOM	2230	ō	ILE	283	14.816	4.543	24.483	1.00 17.19	MTGL
ATOM	2231	N	VAL	284	16.114	2.844	25.200	1.00 17.16	MTGL
ATOM	2232	CA	VAL	284	17.236	3.164	24.321	1.00 15.86	MTGL
ATOM	2233	CB	VAL	284	18.420	2.194	24.554	1.00 16.05	MTGL
ATOM	2234		VAL	284	19.491	2.409	23.491	1.00 14.09	MTGL
ATOM	2235		VAL	284	19.006	2.416	25.956	1.00 14.93	MTGL
MOTA	2236	c	VAL	284	16.797	3.075	22.861	1.00 16.21	MTGL
ATOM	2237	ŏ	VAL	284	17.089	3.963	22.059	1.00 15.26	MTGL
ATOM	2238	N	SER	285	16.086	2.004	22.519	1.00 16.71	MIGL
ATOM	2239	CA	SER	285	15.618	1.813	21.145	1.00 18.87	MTGL
ATOM	2240	СВ	SER	285	14.977	0.429	20.979	1.00 18.71	MTGL
ATOM	2241	OG	SER	285	15.954	-0.595	21.082	1.00 25.57	MTGL
ATOM	2242	Ċ_	SER	285	14.622	2.882	20.697	1.00 18.52	MTGL
ATOM	2243	ŏ	SER	285	14.453	3.101		1.00 19.96	MTGL
MOTA	2244	N	SER	286	13.964	3.544	21.644	1.00 17.61	MTGL
ATOM	2245	CA	SER	286	12.993	4.574		1.00 18.49	MTGL
ATOM	2246	СВ	SER	286	11.970	4.754	22.421	1.00 18.70	MTGL
ATOM	2247	OG	SER	286	12.505	5.533	23.483	1.00 18.21	MTGL
ATOM	2248	c	SER	286	13.686		21.040	1.00 18.76	MTGL
ATOM	2249	ŏ	SER	286	13.043		20.676		MTGL
ATOM	2250	N	VAL	287	15.000		21.235		MTGL
	2251	CA	VAL	287	15.793		21.048	1.00 17.18	MTGL
MOTA	2252	CB	VAL	287	16.866		22.158	1.00 17.69	MTGL
MOTA	2252		1 VAL	287	17.764			1.00 17.29	MTGL
ATOM	2253		2 VAL	287	16.189			1.00 17.29	MTGL
MOTA	2255		VAL		16.493			1.00 17.44	MTGL
ATOM	2255		VAL		16.979			1.00 16.36	MTGL
MOTA			SER		16.546			1.00 18.07	MTGL
MOTA	2257				17.215			1.00 18.93	MTGL
ATOM	2258				17.202				MTGL
ATOM	2259				17.858			1.00 21.05	MTGL
MOTA	2260				18.657				MTGL
MOTA	2261	C	SER	288	10.00				

Fig. 1 cont.

<b>N</b> moM	2262	0	SER	288	19.444	8.498		1.00 18.95	MTGL
ATOM	2262 2263	_	ARG	289	18.984	6,915	17.145	1.00 17.81	MTGL
MOTA		-	ARG	289	20.313	6.311	17.137	1.00 18.49	MTGL
ATOM	2264		ARG	289	21.387	7.347	16.760	1.00 20.78	MTGL
MOTA	2265		ARG	289	21.128	8.067	15.429	1.00 24.72	MTGL
MOTA	2266		ARG	289	22.378	8.761	14.890	1.00 26.86	MTGL
MOTA	2267	CD		289	23.269	7.812	14.225	1.00 31.29	MTGL
MOTA	2268	NE	ARG	289	24.483	8.101	13.758	1.00 32.57	MTGL
ATOM	2269	CZ	ARG		24.981	9.327	13.880	1.00 33.06	MTGL
MOTA	2270	NHI		289	25.200	7.159	13.159	1.00 32.56	MTGL
ATOM	2271	NH2		289	20.687		18.456	1.00 17.41	MTGL
MOTA	2272	C	ARG	289		5.493	18.785	1.00 16.35	MTGL
MOTA	2273	0	ARG	289	21.865	5.173	19.207	1.00 16.31	MTGL
ATOM	2274	N	GLY	290	19.681	4.449	20.442	1.00 16.82	$\mathtt{MTGL}$
MOTA	2275	CA	GLY	290	19.944		19.970	1.00 17.04	MTGL
MOTA	2276	С	GLY	290	20.267	3.042	19.450	1.00 16.17	MTGL
MOTA	2277	0	GLY	290	19.393	2.353	20.159	1.00 17.31	. MTGL
MOTA	2278	N	VAL	291	21.502	2.595		1.00 17.31	MTGL
MOTA	2279	CA	VAL	291	21.893	1.290	19.644	1.00 17.47	MTGL
MOTA	2280	CB	VAL	291	22.951	1.475	18.534	1.00 17.49	MTGL
ATOM	2281		$\mathtt{VAL}$	291	22.387	2.347	17.419	1.00 16.95	MTGL
MOTA	2282	CG2	$_{ m LAV}$	291	24.204	2.125	19.112		MTGL
MOTA	2283	C	VAL	291	22.403	0.194	20.581	1.00 18.18	MTGL
MOTA	2284	0	VAL	291	22.610	-0.933	20.133	1.00 17.39	MTGL
MOTA	2285	N	GLY	292	22.608	0.489	21.861	1.00 18.56	MTGL -
ATOM	2286	CA	GLY	292	23.117	-0.559	22.730	1.00 17.86	MTGL
ATOM	2287	С	GLY	292	22.774	~0.538	24.205	1.00 18.08	
MOTA	2288	Ō	GLY	292	22.404	0.493	24.766	1.00 17.12	MTGL
MOTA	2289	N	LEU	293	22.913	-1.708	24.824	1.00 18.07	MTGL
ATOM	2290	CA	LEU	293	22.653	-1.902	26.246	1.00 18.28	MTGL
MOTA	2291	CB	LEU	293	21.223	-2.404	26.474	1.00 19.14	MTGL
ATOM	2292	CG	LEU	293	20.858	-2.808	27.910	1.00 22.33	MTGL
ATOM	2293		LEU	293	21.047	-1.625	28.842	1.00 23.17	MTGL
MOTA	2294		LEU	293	19,410	-3.278	27.965	1.00 23.54	MTGL
ATOM	2295	C	LEU	293	23.634	-2.952	26.744	1.00 17.77	MTGL
MOTA	2298	0	LEU	293	23.763	-4.009	26.130	1.00 17.95	MTGL
ATOM	2297	Ŋ.	PHE	294	24.322	-2.658	27.847	1.00 16.70	MTGL
ATOM	2298	CA	PHE	294	25.288	-3.586	28.431	1.00 16.53	MTGL
ATOM	2299	CB	PHE	294	26.726	-3.097	28.229	1.00 16.07	MTGL
ATOM	2300	CG	PHE	294	27.199	-3.136	26.800	1.00 16.47	MTGL
	2301		PHE	294	26.792	-2.164	25.890	1.00 16.58	MTGL
MOTA	2302		PHE	294	28.069	-4.137	26.368	1.00 15.29	MTGL
MOTA	2302		PHE	294	27.241	-2.188	24.571	1.00 16.35	MTGL
MOTA	2304		PHE	294	28.523	-4.170	25.050	1.00 15.62	MTGL
MOTA		CZ	PHE	294	28.110	-3.192	24.150	1.00 15.75	MTGL
MOTA	2305 2306		PHE	294	25.046	-3.739		1.00 16.96	MTGL
ATOM		C	PHE	294	25.032	-2.752		1.00 17.04	MTGL
ATOM	2307	0	TYR	295	24.855	-4.977		1.00 16.03	MTGL
ATOM	2308	N		295	24.639	-5.253			MTGL
ATOM	2309	CA	TYR		23.000	-6 582	31 963	1.00 14.47	MTGL
MOTA	2310	CB	TYR	295		-6.755	33.344	1.00 14.21	MTGL
ATOM	2311	CG	TYR	295	23.323	-6.312			MTGL
ATOM	2312	CD		295	22.033 21.512	-6.421			MTGL
ATOM	2313		1 TYR						MTGL
ATOM	2314		2 TYR		24.080	-7.316			MTGL
MOTA	2315				23.566	-7.431			MTGL
MOTA	2316		TYR		22.284	-6.979			MTGL
ATOM	2317		TYR		21.784	-7.058			MTGL
ATOM	2318	C	TYR		26.033	-5.346			MTGL
MOTA	2319	0	TYR	295	26.932	-5.933	31.814	1.00 15.00	MOIM

Fig. 1 cont.

	2222		מ מיזיי	296	26.228	-4.778	33,594	1.00 14.56	MTGL
MOTA	2320	N	TRP	296	27.559	-4.829	34.195	1.00 15.23	MTGL
ATOM	2321	CA	TRP	296	27.847	-3.541	34.984	1.00 14.28	MTGL
ATOM	2322	CB	TRP		29.306	-3.370	35.309	1.00 15.53	MTGL
ATOM	2323	CG	TRP	296	29.918	-3.408	36.611	1.00 16.19	MTGL
MOTA	2324	CD2	TRP	296	31.309	-3.221	36.424	1.00 15.45	MTGL
MOTA	2325	CE2	TRP	296		-3.583	37.916	1.00 16.72	MTGL
MOTA	2326	CE3		296	29.428	-3.168	34.418	1.00 15.37	MTGL
MOTA	2327	CD1		296	30.321	-3.100	35.079	1.00 15.66	MIGL
ATOM	2328	NE1		296	31.526		37.495	1.00 15.00	MTGL
ATOM	2329		TRP	296	32.219	-3.201	38.985	1.00 16.55	MTGL
ATOM	2330		TRP	296	30.334	~3.564	38.763	1.00 16.36	MTGL
MOTA	2331	CH2	TRP	296	31.715	-3.375		1.00 14.61	MTGL
ATOM	2332	С	TRP	296	27.842	-6.029	35.097	1.00 15.45	MTGL
ATOM	2333	0	TRP	296	27.174	-6.224	36.114	1.00 13.43	MTGL
ATOM	2334	N	GLU	297	28.835	-6.826	34.702		MTGL
MOTA	2335	CA	GLU	. 297	29.298	-7.977	35.479	1.00 14.59	MTGL
ATOM	2336	CB	GLU	297	30.125	-7.465	36.661	1.00 13.64	MTGL
MOTA	2337	CG	GLU	297	31.453	-6.849	36.261	1.00 14.27	MTGL
ATOM	2338	CD	GLU	297	32.506	-7.896	35.947	1.00 13.45	
MOTA	2339	OE1	GLU	297	32.176	-9.102	35.991	1.00 12.29	MTGL
ATOM	2340	OE2	GLU	297	33.661	-7.510	35.660	1.00 14.90	MTGL
ATOM	2341	С	GLU	297	28.245	-8.952	36.000	1.00 15.16	MTGL
ATOM	2342	Ó	GLU	297	28.177	-9.219	37.205	1.00 15.61	MTGL
ATOM	2343	N	PRO	298	27.436	-9.529	35.100	1.00 14.59	MTGL
ATOM	2344	CD	PRO	298	27.545	-9.487	33.631	1.00 12.84	MTGL
MOTA	2345	CA	PRO	298	26.395	-10.474	35.517	1.00 14.70	MTGL
MOTA	2346	CB	PRO	298	25.651		34.217	1.00 13.52	MTGL
ATOM	2347	CG	PRO	298	26.765	-10.716	33.213	1.00 12.86	MTGL
ATOM	2348	c	PRO	298	26.897	-11.774	36.158	1.00 14.86	MTGL
ATOM	2349	ō	PRO	298	26.159	-12.424	36.901	1.00 14.01	MTGL
ATOM	2350	Ŋ	ALA	299	28.143	-12.147	35.875	1.00 15.30	MTGL
ATOM	2351	CA	ALA	299	28.689	-13.397	36.396	1.00 16.12	MTGL
ATOM	2352	CB	ALA	299	29.321	-14.184	35.245	1.00 16.45	MTGL
ATOM	2353	Č	ALA	299	29.684	-13.297	37.551	1.00 16.40	MTGL
ATOM	2354	ŏ	ALA	299	30.281	-14.303	37.934	1.00 16.31	MTGL
MOTA	2355	N	TRP	300		-12.104	38.111	1.00 16.53	MTGL
ATOM	2356	CA	TRP	300		-11.911	39,218	1.00 16.99	MTGL
MOTA	2357	CB	TRP	300	31.205	-10.438	39.300	1.00 15.26	MTGL
ATOM	2358	ÇG	TRP	300	32.518	-10.195	39.960	1.00 16.30	MTGL
ATOM	2359	CD2		300	33.248		39.982	1.00 14.96	MTGL
ATOM	2360	CE		300	34.440		40.697	1.00 14.93	MTGL
MOTA	2361	CE:		300	33.007		39.463	1.00 15.40	MTGL
ATOM	2362		TRP	300		-11.099	40.648	1.00 14.90	MTGL
	2363	NE:	-	300		-10.508	41.092	1.00 16.48	MTGL
MOTA			2 TRP	300	35.398			1.00 13.85	MTGL
MOTA	2364			300	33.960			1.00 13.88	MTGL
ATOM	2365	CZ:	2 TRP	300	35.143			1.00 15.26	MTGL
ATOM	2366					-12.347			MTGL
ATOM	2367	C	TRP	300 300		-11.522	41.423	1.00 16.66	MTGL
MOTA	2368	0	TRP	300	29.903	-13.645			MTGL
MOTA	2369	N	ILE			-13.043			MTGL
MOTA	2370	CA	ILE	301		-14.166 -15.655			MTGL
ATOM	2371	CB	ILE	301		-15.812			MTGL
ATOM	2372		2 ILE	301					MTGL
MOTA	2373		1 ILE			3 -16.496			MTGL
atom	2374		l ILE	301	29.858	-17.985			MTGL
ATOM	2375		ILE		29.973	-13.980	43.203		MTGL
ATOM	2376		ILE			-14.022			MTGL
ATOM	2377	N	HIS	302	31.287	7 -13.768	43.189	T.00 TA'1A	1.11.077

Fig. 1 cont.

		~~		302	32.016 -	13 555	44.441	1.00 21.73	MTGL
MOTA	2378		HIS		33.464 -	14.042	44.317	1.00 22.38	MTGL
ATOM	2379		HIS	302	33.603 -	15 529	44.396	1.00 24.09	MTGL
ATOM	2380		HIS	302	33.254 -	16 405	45.368	1.00 25.41	MTGL
ATOM	2381	CD2		302	34.154 -	16 202	43.382	1.00 25.82	MTGL
MOTA	2382	NDI		302	34.137 -	17 55Ω	43.724	1.00 26.05	MTGL
MOTA	2383	CE1		302	33.596 ~	17 650	44.924	1.00 26.28	MTGL
ATOM	2384	NE2		302	32.002 -	12 005	44.857	1.00 21.31	MTGL
MOTA	2385		HIS	302	32.609 -	11 707	45.854	1.00 22.67	MTGL
MOTA	2386		HIS	302	32.609 -	11.707	44.079	1.00 20.90	MTGL
ATOM	2387		ASN	303	31.303 -		44.337	1.00 20.21	MTGL
MOTA	2388		ASN	303		-9.831		1.00 20.27	MTGL
ATOM	2389		ASN	303		-9.074	43.473	1.00 20.27	MTGL
ATOM	2390	CG	ASN	303	32.170	-7.573	43.706	1.00 22.04	MTGL
MOTA	2391	OD1		303	31.977	-7.118	44.828		MTGL
ATOM .	2392	ND2	ASN	303	32.380	~6.799	42.643	1.00 19.16	MTGL
ATOM	2393	С	ASN	303	29.752	-9.467	43.946	1.00 20.34	
MOTA	2394	0	ASN	303	29.508	-8.488	43.233	1.00 18.25	MTGL
ATOM	2395	N	ALA	304	28.820 -	-10.284	44.432	1.00 19.57	MTGL
ATOM	2396	CA	ALA	304	27.395 -	-10.180	44.134	1.00 19.48	MTGL
ATOM	2397	CB	ALA	304	26.612 -		45.017	1.00 18.17	MTGL
ATOM	2398	С	ALA	304	26.731	-8,813	44.182	1.00 19.61	MTGL
ATOM	2399	0	ALA	304	25.909	-8.505	43.323	1.00 20.70	MTGL
ATOM	2400	·N	ASN	305	27.050	-7.999	45.181	1.00 18.88	MTGL
MOTA	2401	CA	ASN	305	26.424	-6.685	45.271	1.00 19.31	MTGL
ATOM	2402	CB	ASN	305	26.580	-6.114	46.683	1.00 19.61	MTGL
ATOM	2403	CG	ASN	305 ^	28.024	-5.847	47.048	1.00 20.60	MTGL
ATOM	2404		ASN	305	28.868	-6.747	47.014	1.00 21.53	MTGL
ATOM	2405		ASN	305	28.318	-4.606	47.403	1.00 21.29	MTGL
ATOM	2406	C	ASN	305	27.018	-5.723	44.240	1.00 19.61	MTGL
ATOM	2407	ŏ	ASN	305	26.522	-4.611	44.041	1.00 19.33	MTGL
ATOM	2408	Ŋ	LEU	306	28.088	-6.160	43.587	1.00 18.26	MTGL
ATOM	2409	CA	LEU	306	28.747	-5.359	42.563	1.00 18.47	MTGL
MOTA	2410	CB	LEU	306-	27.919	-5.384	41.270	1.00 17.67	MTGL
ATOM	2411	CG	LEU	306	27.771	-6.764	40.612	1.00 18.35	MTGL
ATOM	2412		LEU	306	26.888	-6.670	39.372	1.00 16.49	MTGL
MOTA	2413		LEU	306	29.144	-7.300	40.238	1.00 16.40	MTGL
ATOM	2414	. C	LEU	306	28.994	-3.915	42.990	1.00 19.28	MTGL
	2415	ő	LEU	306	28.698	-2.981	42.241	1.00 19.04	MTGL
ATOM	2415	N	GLY	307	29.529	-3.740	44.196	1.00 18.62	MTGL
ATOM			GLY	307	29.828		44.700	1.00 18.44	$\mathtt{MTGL}$
MOTA	2417	CA C	GLY	307	28.657	-1.530	45.092	1.00 18.36	MTGL
MOTA	2418	Ö	GLY	307	28.866	-0.379	45.466	1.00 18.04	MTGL
MOTA	2419		SER	308	27.435	-2.047	45.020	1.00 17.93	
MOTA	2420	N CT	SER	308 -	26.256	-1.256	45.380	1.00 17.81	
MOTA	2421	CA	SER	308	25.134	-1.480	44.361	1.00 16.84	MTGL
ATOM	2422	CB	SER	308	24.555	-2.759	44.528	1.00 15.76	
ATOM	2423	OG		308	25.756	-1.651	46.762	1.00 18.10	
MOTA	2424	C	SER		26.282	-2.585	47.361	1.00 18.30	
MOTA	2425	0	SER	308		-0.947	47.250	1.00 18.76	
MOTA	2426	N	SER	309	24.735	-1.220	48.560	1.00 20.76	MTGL
ATOM	2427	CA	SER	309	24.157	0.022	49.092	1.00 21.48	
MOTA	2428	CB	SER	309	23.424		48.283	1.00 22.88	
MOTA	2429	OG	SER	309	22.304	0.358		1.00 22.16	
ATOM	2430	C	SER	309	23.193	-2.404	48.517	1.00 23.34	
ATOM	2431	0	SER	309	22.754	-2.899	49.560	1.00 22.36	
MOTA	2432	N	CYS	310	22.852	-2.846	47.312		
MOTA	2433		CYS	310	21.954	-3.987	47.159		
ATOM	2434		CYS	310	22.784	-5.265	47.300		
ATOM	2435	0	CYS	310	23.935	-5.300	46.877	1.00 25.45	5 MTGL

Fig. 1 cont.

		~~	ava	27.0	21.275	-3.945	45.793	1.00 23.30	MTGL
ATOM	2436	-	CYS	310	19.871	-2.792	45.648	1.00 24.32	MTGL
MOTA	2437		CYS	310		-6.309	47.877	1.00 21.14	MTGL
MOTA	2438	-	ALA	311	22.197	-7.564	48.110	1.00 20.13	MTGL
ATOM	2439		ALA	311	22.903		49.052	1.00 20.15	MTGL
MOTA	2440	CB	ALA	311	22.076	-8.449		1.00 19.87	MTGL
ATOM	2441	C.	ALA	311	23.335	-8.383	46.894		MTGL
ATOM	2442	0	ALA	311	24.442	-8.915	46.875	1.00 18.96	MTGL
MOTA	2443	N	ASP	312	22.482	-8.502	45.882	1.00 18.99	
ATOM	2444		ASP	312	22.849	-9.313	44.723	1.00 19.21	MTGL
ATOM	2445		ASP	312	22.346	-10.747	44.931	1.00 19.01	MTGL
MOTA	2446	ĊĠ	ASP	312	22.949	-11.733	43.946	1.00 19.92	MTGL
ATOM	2447	OD1		312	23.450	-11.305	42.884	1.00 19.68	MTGL
ATOM	2448	OD2		312	22.908	-12.948	44.230	1.00 20.69	MTGL
MOTA	2449	C	ASP	312	22.310	-8.772	43.403	1.00 18.27	MTGL
ATOM	2450	ŏ	ASP	312	21.098	-8.692	43.205	1.00 18.94	MTGL
	2451	N	ASN	313	23.222	-8.418	42.500	1.00 17.28	MTGL
ATOM		CA	ASN	313	22.855	-7.892	41.187	1.00 17.18	MTGL
ATOM	2452		ASN	313	23.478	-6.507	40.962	1.00 16.90	MTGL
ATOM	2453	CB	ASN	313	22.860	-5.440	41.835	1.00 17.53	MTGL
ATOM	2454	CG		313	21.636	-5.293	41.879	1.00 20.07	MTGL
ATOM	2455		ASN		23.704	-4.677	42.529	1.00 16.34	MTGL
ATOM	2456		ASN	313	23.305		40.053	1.00 17.15	$\mathtt{MTGL}$
ATOM	2457	C	ASN	313	23.190		38.881	1.00 17.24	$\mathtt{MTGL}$
ATOM	2458	0	ASN	313	23.190		40.391	1.00 15.74	MTGL
ATOM	2459	Ŋ	THR	314		-10.903	39.365	1.00 15.54	MTGL
MOTA	2460	CA	THR	314	24.209	-11.977	39.953	1.00 15.83	MTGL
MOTA	2461	CB	THR	314	23.220	-12.779	40.894	1.00 16.12	MTGL
MOTA	2462		THR	314	24.502	-11.322	40.651	1.00 14.76	MTGL
MOTA	2463		THR	314	20.410	-11.604	38.657	1.00 16.42	MTGL
ATOM	2464	č	THR	314	23.130	-11.525	39.087	1.00 15.23	MTGL
MOTA	2465	0	THR	314	21.312	-12.273	37.555	1.00 16.30	MTGL
MOTA	2466	И	MET	315	23,433	-13.005	36.776	1.00 17.57	MTGL
MOTA	2467	CA	MET	315	22.430	-12.447	35.350	1.00 16.92	MTGL
MOTA	2468	CB	MET	315		-10.997	35.281	1.00 16.10	MTGL
MOTA	2469	CG	MET	315		-10.343	33.592	1.00 18.97	MTGL
ATOM	2470	SD	MET	315			33.083	1.00 14.39	MTGL
ATOM	2471	CE	MET	315		-10.916 -14.492	36.753	1.00 17.49	MTGL
MOTA	2472	С	MET	315			35.871	1.00 17.40	MTGL
ATOM	2473	0	MET	315		-15.234 -14.905	37.736	1.00 17.70	MTGL
MOTA	2474	N	PHE	316			37.879	1.00 18.51	MTGL
MOTA	2475	CA	PHE	316		-16.291	37.482	1.00 16.98	MTGL
MOTA	2476	CB	PHE	316		16.451		1.00 17.56	MTGL
ATOM	2477	CG	PHE	316		) -16.485 5 -15.337	35.220	1.00 17.13	MTGL
ATOM	2478		PHE	316		1 -17.671		1.00 16.95	MTGL
MOTA	2479		PHE	316				1.00 17.76	MTGL
MOTA	2480		PHE	316		5 -15.370 5 -17.717			MTGL
ATOM	2481		PHE	316					MTGL
ATOM	2482	CZ	PHE	316	20.214	2 -16.566		1.00 19.70	MTGL
MOTA	2483	Ç	PHE	316	23.89.	1 -16.679	39.344		MTGL
ATOM	2484	0	PHE	316	23,980	0 -15.825	39.598	1.00 19.30	MTGL
ATOM	2485		SER	317		9 -17.963			MTGL
MOTA	2486		SER	317		5 -18.444			MTGL
MOTA	2487	CB	SER	317	22.89	4 -19.853 2 -20 799			MTGL
MOTA	2488	OG	SER	317		2 - 20.798			MTGL
MOTA	2489		SER	317		0 -18.479			MTGL
MOTA	2490		SER	317	25.89	5 -18.352			MTGL
ATOM	2491		GLN	318		7 -18.659			MTGL
MOTA	2492			318		4 -18.711			MTGL
ATOM	2493	CB	GLN	318	25.81	3 -18.649	45.186	1.00 23.00	1,100

Fig. 1 cont.

		~~	C7 N3	318	25.363 -17.254 45.625 1.00	24.34	MTGL
MOTA	2494	CG	GLN	318		25.12	MTGL
MOTA	2495		GLN	318		27.51	MTGL
MOTA	2496	OE1				23.16	MIGL
MOTA	2497	NE2		318		22.71	MTGL
MOTA	2498	С	GLN	318		24.10	MTGL
ATOM	2499	0	GLN	318		22.97	MTGL
MOTA	2500	N	SER	319		23.61	MTGL
MOTA	2501	CA	SER	319	27.022 22.01.	24.83	MTGL
ATOM	2502	CB	SER	319	20.42	28.30	MTGL
ATOM	2503	OG	SER	319		23.21	MTGL
ATOM	2504	C	SER	319		23.75	MTGL
MOTA	2505	0	SER	319	20.200	22.56	MTGL
ATOM	2506	N	ĠLY	320		22.10	MTGL
MOTA	2507	CA	GLY	320	27.790 20.100 00.00		MTGL
ATOM	2508	С	GLY	320	20.002	22.30	MTGL
ATOM	2509	0	GLY	320	2,1202	22.30	
ATOM	2510	N	GLN	321	20.002 02.002	21.21	MTGL
ATOM	2511	CA	GLN	321		21.36	MTGL
MOTA	2512	CB	GLN	321	20,032 00.124	23.27	MTGL
ATOM	2513	CG	GLN	321		24.43	MTGL
ATOM	2514	CD	GLN	321	22.000	26.48	MTGL
MOTA	2515		GLN	321		27.39	MTGL
ATOM	2516		GLN	321		27.02	MTGL
ATOM	2517	C	GLN	321	23.826 -20.121 36.483 1.00	20.04	MTGL
MOTA	2518	ŏ	GLN	321		19.56	MTGL
ATOM	2519	N	ALA	322	23.755 -19.939 35.172 1.00	20.60	MTGL
ATOM	2520	CA	ALA	322	23 028 -18 817 34 596 1 00	20.07	MTGL
ATOM	2521	CB	ALA	322	23.129 -18.864 33.079 1.00	18.41	MTGL
MOTA	2522	C	ALA	322	21 565 -18.855 35.017 1.00	20.05	MTGL
ATOM	2523	ŏ	ALA	322	20.921 -19.901 34.945 1.00	19.07	MTGL
ATOM	2524	N	LEU	323	21.052 -17.713 35.464 0.50	19.28	MTGL
	2525	CA	LEU	323	19.658 -17.611 35.878 0.50	19.33	MTGL
ATOM	2526	CB	LEU	323	19.470 -16.426 36.830 0.50	18.12	MTGL
MOTA	2527	CG	LEU	323	20.241 -16.493 38.152 0.50	17.16	MTGL
MOTA	2528		LEU	323		16.83	MTGL
ATOM	2529		LEU	323		16.13	MTGL
MOTA			LEU	323		19.86	MTGL
ATOM	2530	C	LEU	323		19.75	MTGL
ATOM	2531	0		324		21.01	MTGL
MOTA	2532		SER	324		21.34	MTGL
MOTA	2533	CA	SER			21.65	MTGL
ATOM	2534	CB	SER	324	14.713 -16.887 35.202 1.0	0 22.41	MTGL
ATOM	2535	OG	SER	324		0 21.33	MTGL
MOTA	2536	Č	SER	324		0 20.59	MTGL
MOTA	2537	0	SER	324		0 20.04	MTGL
ATOM	2538	N	SER	325	10.200	0 20.07	MTGL
MOTA	2539	CA	SER	325	10.001 10.000 00	0 19.69	MTGL
MOTA	2540	CB	SER	325	21122	0 17.73	MTGL
ATOM	2541	OG	SER	325		0 20.16	MTGL
ATOM	2542		SER	325	10.012 10.010	0 19.87	MTGL
MOTA	2543	0	SER	325		0 19.54	MTGL
ATOM	2544		LEU	326	19.010 19.000 00000	0 19.34	MTGL
ATOM	2545	CA	LEU	326			MTGL
MOTA	2546	CB	LEU			0 20.49	MTGL
MOTA	2547	CG	LEU	326		0 22.10	
ATOM	2548	CD	1 LEU		201120 = 1011	0 21.95	MTGL
MOTA	2549		2 LEU			0 22.81	MTGL
ATOM	2550		LEU			0 19.72	MTGL
ATOM	2551		LEU		20.094 ~13.655 28.754 1.0	0 19.08	MTGL

Fig. 1 cont.

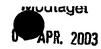
	0550	**	SER	327	18.439 -15	.015	29.412	1.00	18.98	MTGL
ATOM	2552		SER	327	17.875 -15		28.067	1.00	18.71	MTGL
MOTA	2553	_		327	16.861 -16		28.023	1.00	17.52	$\mathtt{MTGL}$
MOTA	2554		SER	327	15.740 -15		28.825	1.00	16.77	MTGL
ATOM	2555		SER		17.191 -13		27.585	1.00	18.81	MTGL
ATOM	2556		SER .	327	16.698 -13	795	26.459		18.63	MTGL
ATOM	2557	0	SER	327	17.140 -12		28.440		18.22	MTGL
MOTA	2558	N	VAL	328	16.517 -11	573	28.066		18.51	MTGL
MOTA	2559	CA	VAL	328			29.223		19.11	MTGL
MOTA	2560	CB	VAL	328	16.590 -10	177	29.509		17.14	MTGL
MOTA	2561	CG1		328	18.046 -10	.304	28.868		19.04	MTGL
ATOM	2562	CG2		328			26.839		19.25	MTGL
ATOM	2563	С	VAL	328	17.210 -10	205	26.039		18.81	MTGL
MOTA	2564	0	VAL	328	16.589 -10	.200	26.685		20.22	MTGL
MOTA	2565	N	PHE	329	18.498 -11	.2/3			22.10	MTGL
MOTA	2566	CA	PHE	329	19.258 -10	. 752	25.550		21.20	MTGL
ATOM	2567	CB	PHE	329	20.752 -10		25.774		21.71	MTGL
ATOM	2568	CG	PHE	329	21.307 -10		26.929		21.66	MTGL
MOTA	2569	CD1	PHE	329		.842	26.814		20.67	MTGL
ATOM	2570	CD2	PHE	329	21.551 -10		28.151	1.00	20.07	MTGL
ATOM	2571	CE1	PHE	329		.099	27.901	1.00	22.16	MTGL
ATOM	2572	CE2	PHE	329	22.003 -10		29.240	1.00	22.03	MTGL
ATOM	2573	CZ	PHE	329		3.728	29.114	1.00	22.57	MTGL
MOTA	2574	C	PHE	329		L.340	24.212	1.00	23.27	
ATOM	2575	Ō	PHE	329	19.267 -10	).904	23.152		23.56	MTGL
ATOM	2576	N	GLN	330	17.927 -12	2.326	24.267		23.16	MTGL
ATOM	2577	CA	GLN	330	17.402 -12		23.058		24.83	MTGL
ATOM	2578	СВ	GLN	330	16.994 -14	1.403	23.333		25.48	MTGL
MOTA	2579	CG	GLN	330	18.138 -15	5.371	23.573		25.89	MTGL
ATOM	2580	CD	GLN	330	17.648 -10	6.773	23.894		27.09	Mīgl
ATOM	2581		GLN	330	18.390 -1	7.748	23.750	1.00	29.08	MTGL
ATOM	2582		GLN	330	16.400 -1		24.343		24.64	MTGL
ATOM	2583	c	GLN	330	16.157 -13	2.198	22.596		25.46	. MTGL
MOTA	2584	ŏ	GLN	330	15.651 -1	2.439	21.502	1.00	25.45	MTGL
MOTA	2585	N	ARG	331	15.669 -1	1.282	23.426	1.00	25.05	MTGL
ATOM	2586	CA	ARG	331	14.443 -1	0.573	23.094	1.00	25.37	MTGL
ATOM	2587	CB	ARG	331	13.356 -1		24.087		24.60	MTGL
	2588	ÇG	ARG	331	13.223 -1		24.246	1.00	25.96	MTGL
MOTA	2589	CD	ARG	331	12.110 -1		25.220	1.00	26.44	MTGL
MOTA		NE	ARG	331	12.400 -1	2.493	26.600	1.00	27.25	MTGL
ATOM	2590	CZ	ARG	331	13.123 -1	3.218	27.451	1.00	27.98	MTGL
MOTA	2591		. ARG	331	13.637 -1		27.073		26.83	MTGL
MOTA	2592		ARG	331	13.329 -1	2.777	28.683	1.00	26.92	MTGL
MOTA	2593		ARG	331		9.049	23.017		25.38	MTGL
MOTA	2594	C		331		8.391	23.085	1.00	25.25	MTGL
ATOM	2595	0	ARG	332		8.487	22.863		25.52	$\mathtt{MTGL}$
ATOM	2596	N	ILE			7.035	22.779	1.0	26.69	$\mathtt{MTGL}$
MOTA	2597	CA	ILE	332		6.459	24.049		0 26.08	MTGL
ATOM	2598	CB	ILE	332		6.765	25.269	1.0	0 25.81	MTGL
MOTA	2599		S I LE	332		-7.047	24.224		0 25.06	MTGL
MOTA	2600		LILE	332		-7.047 -6.506			0 23.51	MTGL
ATOM	2601		LILE	332				_	0 27.88	MTGL
MOTA	2602		ILE	332		-6.599		_	0 28.65	MTGL
MOTA	2603		ILE	332		-7.485			0 30.38	MTGL
MOTA	2604	OX.	I ITE	332	16.787 -	-5.372	41.344	1.0	5 50.50	
END										

Fig. 1 cont.



				•			
HEADER			•	6 047	74 240 114 849	HIGL 1.00 27.43	HIGL
MOTA	1 CB	ALA	1	6.247	74.348 114.849 72.458 113.617	1.00 26.21	HIGL
ATOM	2 C	ALA	1	7.283	72.438 113.617	1.00 26.69	HIGL
MOTA	3 0	ALA	1	6.683 7.237	74.771 112.633	1.00 26.59	HIGL
MOTA	4 N	ALA	1	7.343	73.961 113.863	1.00 26.86	HIGL
ATOM	5 CA	ALA	1	7.883	71.693 114.524	1.00 24.15	HIGL
MOTA	6 N	LEU	2	7.883	70.244 114.405	1.00 22.16	HIGL
ATOM	7 CA	LEU	2	8.883	69.700 115.498	1.00 21.06	HIGL
ATOM	8 CB	LEU	2 2	10.274	70.334 115.565	1.00 20.32	HIGL
ATOM	9 CG	LEU	2	10.966	69.921 116.848	1.00 19.78	HIGL
ATOM	10 CD1	LEU	2	11.076	69.921 114.346	1.00 20.05	HIGL
ATOM	11 CD2 12 C	LEU LEU	2	6.663	69.471 114.429	1.00 22.53	HIGL
ATOM		LEU	2	5.748	69.767 115.202	1.00 23.10	HIGL
ATOM	13 O 14 N	GLN	3	6.597	68.456 113.576	1.00 21.51	HIGL
MOTA	15 CA	GLN	3	5.430	67.601 113.493	1.00 20.06	HIGL
ATOM ATOM	16 CB	GLN	3	5.435	66.837 112.175	1.00 18.80	HIGT
ATOM	17 CG	GLN	3	4.157	66.084 111.909	1.00 19.14	HIGL
ATOM	18 CD	GLN	3	4.246	65.213 110.680	1.00 19.73	HIGL
ATOM	19 OE1	GLN	3	4.884	65.577 109.689	1.00 21.27	HIGL
ATOM	20 NE2	GLN	3	3.594	64.062 110.728	1.00 18.71	HIGL
ATOM	21 C	GLN	3	5.504	66.609 114.644	1.00 19.78	HIGL
ATOM	22 0	GLN	3	4.513	66.342 115.324	1.00 20.14	HIGL
ATOM	23 N	TYR	4	6.696	66.060 114.849	1.00 19.50	HIGL
ATOM	24 CA	TYR	4	6.920	65.083 115.902	1.00 19.32	HIGL
ATOM	25 CB	TYR	4	7.614	63.849 115.328	1.00 18.96	HIGL
ATOM	26 CG	TYR	4	6.913	63.222 114.145	1.00 19.19	HIGL
ATOM	27 CD1	TYR	4	5.639	62.669 114.271	1.00 19.50	HIGL
ATOM	28 CE1	TYR	4	5.019	62.033 113.199	1.00 18.39	$ ext{HIGL}$
MOTA	29 CD2	$\pi Y R$	4	7.546	63.131 112.909	1.00 19.30	HIGL
ATOM	30 CE2	TYR	4	6.935	62.497 111.831	1.00 19.42	HIGL
MOTA	31 CZ	TYR	4	5.672	61.947 111.984	1.00 19.38 1.00 18.91	HIGL
ATOM	32 OH	TYR	4	5.083	61.288 110.922	1.00 18.91	HIGL
ATOM	33 C	TYR	4	7.790	65.686 117.000 66.022 116.776	1.00 19.37	HIGL
ATOM	34 O	TYR	4	8.954 7.220	65.845 118.185	1.00 19.13	HIGL
ATOM	35 N	LYS	5	7.220	66.388 119.293	1.00 19.83	HIGL
ATOM	36 CA	LYS	5 5	7.666	67.874 119.495	1.00 21.28	HIGL
ATOM	37 CB	LYS	5	6.198	68.219 119.599	1.00 23.14	HIGL
MOTA	38 CG	LYS LYS	5	6.031	69.730 119.695	1.00 25.10	HIGL
MOTA	39 CD 40 CE	LYS	5	4.563	70.143 119.714	1.00 25.68	HIGL
ATOM	40 CE 41 NZ	LYS	5	4.438	71.621 119.884	1.00 27.35	HIGL
MOTA MOTA	42 C	LYS	5	7.661	65.589 120.539	1.00 19.09	HIGL
ATOM	43 0	LYS	5	6.537	65.616 121.043	1.00 20.34	HIGL
MOTA	44 N	GLY	6	8.653	64.858 121.027	1.00 17.54	HIGL
ATOM	45 CA	.GLY	6	8.428	64.050 122.203	1.00 16.41	HIGL
MOTA	46 C	GLY	6	9.685	63.574 122.897	1.00 15.75	HIGL
MOTA	47 0	GLY	6	10.779	64.112 122.698	1.00 15.49	HIGL
ATOM	48 N	VAL	7	9.518	62.548 123.721		HIGL
MOTA	49 CA	VAL	7	10.623			HIGL
ATOM	50 CB	VAL	7	10.518	62.373 125.963		HIGL
MOTA	51 CG1		7	10.337			HIGL
ATOM	52 CG2	VAL	7	9.361		1.00 14.47	HIGL
ATOM	53 C	VAL	7	10.629			HIGL HIGL
ATOM	54 O	VAL	7	9.650	59.863 123.979		HIGL
MOTA	55 N	ASP	8	11.753		1.00 13.51	HIGL
MOTA	56 CA	ASP	8	11.863			HIGL
MOTA	57 CB	ASP	8	13.263		3 1.00 13.57 3 1.00 13.68	HIGL
ATOM	58 CG	ASP	8	13.354			HIGL
MOTA	59 OD1		8	12.912	55.814 125.353		HIGL
ATOM	60 OD2		8	13.861	55.967 123.373		HIGL
MOTA	61 C	ASP	8	11.626			HIGL
ATOM	62 0	ASP	8	12.391			HIGL
ATOM	63 N	TRP	9	10.562			HIGL
ATOM	64 CA	TRP	9	10.207	J1,200 120.03		

Fig. 2



				4	7/174	PVS	
ATOM	65 CB	TRP	9	8.822	57.889 128.324	1.00 11.91	HIGL
MOTA	66 CG	TRP	9	7.684	57.044 127.823	1.00 12.26	HIGL
ATOM	67 CD2	TRP	9	6.406	56.867 128.448	1.00 12.11	HIGL
MOTA MOTA	68 CE2 69 CE3	TRP	9 9	. 5.670 5.809	55.963 127.647 57.383 129.609	1.00 12.19 1.00 11.70	HIGL HIGL
ATOM	70 CD1	TRP	9	7.668	56.268 126.696	1.00 11.92	HIGL
MOTA	71 NE1	TRP	9	6.4.66	55.614 126.586	1.00 11.76	HIGL
ATOM	72 CZ2	TRP	9	4.365	55.562 127.968	1.00 11.52	HIGL
ATOM	73 CZ3	TRP	9	4.510	56.986 129.930	1.00 11.57	HIGL
ATOM ATOM	74 CH2 75 C	TRP TRP	9 9	3.804 10.212	56.085 129.111 55.798 128.440	1.00 11.64 1.00 14.10	HIGL HIGL
ATOM	76 O	TRP	9	9.551	55.392 129.392	1.00 15.49	HIGL
MOTA	77 N	SER	10	10.984	55.002 127.713	1.00 14.17	HIGL
ATOM	78 CA	SER	10	11.051	53.561 127.939	1.00 14.00	HIGL
MOTA MOTA	79 CB 80 OG	SER SER	10 10	12.154 11.946	52.958 127.056 53.282 125.685	1.00 14.22 1.00 12.67	HIGL
ATOM	81 C	SER	10	11.232	53.095 129.385	1.00 13.46	HIGL
ATOM	82 O	SER	10	10.652	52.096 129.794	1.00 13.12	HIGL
ATOM	83 N	SER	11	12.021	53.821 130.162	1.00 13.49	HIGL
MOTA	84 CA	SER	11	12.281	53.437 131.542	1.00 13.65 1.00 12.96	HIGL
ATOM ATOM	85 CB 86 OG	SER SER	11 11	13.490 13.175	54.200 132.051 55.576 132.142	1.00 12.96	HIGL HIGL
ATOM	87 C	SER	11	11.134	53.664 132.524	1.00 15.06	HIGL
ATOM	88 O	SEŖ	11	11.192	53.198 133.667	1.00 15.59	HIGL
MOTA	89 N	JAV	12	10.090	54.357 132.089	1.00 15.52	HIGL
ATOM ATOM	90 CA 91 CB	VAL VAL	12 12	8.987 7.793	54.682 132.983 55.248 132.197	1.00 16.34 1.00 16.01	HIGL HIGL
ATOM	92 CG1	VAL	12	7.264	54.205 131.248	1.00 16.29	HIGL
ATOM	93 CG2	VAL	. 12	6.714	55.720 133.159	1.00 15.28	HIGL
MOTA	94 C	VAL	12	8.485	53.594 133.945	1.00 17.29	HIGL
ATOM ATOM	95 O 96 N	VAL MET	12	8.361	53.855 135.143	1.00 18.04	HIGL
ATOM	97 CA	MET	13 13	8.197 7.695	52.390 133.457 51.346 134.355	1.00 17.84 1.00 17.96	HIGL HIGL
ATOM	98 CB	MET	13	7.044	50.203 133.568	1.00 17.95	HIGL
MOTA	99 CG	MET	13	5.703	50.579 132.968	1.00 19.53	HIGL
ATOM	100 SD	MET	13	4.678	49.147 132.593	1.00 23.13	HIGL
MOTA MOTA	101 CE 102 C	MET MET	13 13	5.559 8.756	48.452 131.185 50.788 135.290	1.00 23.08° 1.00 17.76	HIGL HIGL
ATOM	103 0	MET	13	8.456	50.415 136.420	1.00 17.26	HIGL
MOTA	104 N	VAL	14	9.994	50.723 134.817	1.00 17.91	HIGL
ATOM	105 CA	VAL	14	11.082	50.225 135.640	1.00 17.21	HIGL
ATOM ATOM	106 CB 107 CG1	VAL VAL	14 14	12.413	50.169 134.845 49.837 135.761	1.00 16.85 1.00 13.37	HIGL HIGL
ATOM	108 CG2	VAL	14	12.311	49.128 133.741	1.00 15.66	HIGL
MOTA	109 C	$\cdot VAL$	14	11.212	51.187 136.809	1.00 17.76	HIGL
ATOM	110 0	VAL	14	11.455	50.774 137.945	1.00 18.17	HIGL
ATOM ATOM	111 N 112 CA	GLU	15 15	11.031 11.120	52.473 136.533 53.476 137.586	1.00 18.10 1.00 19.10	HIGL HIGL
MOTA	113 CB	GLU	15	11.207	54.881 136.991	1.00 19.32	HIGL
MOTA	114 CG	GLU	15	12.554	55.178 136.365	1.00 20.08	HIGL
ATOM	115 CD	GLU	15	13.676	55.158 137.383	1.00 21.57	HIGL
MOTA MOTA	116 OE1 117 OE2	GLU	15 15	13.838	54.131 138.076	1.00 22.32	HIGL
ATOM	117 GEZ	GLU GLU	15	14.398 9.937	56.171 137.492 53.387 138.539	1.00 22.71 1.00 19.39	HIGL HIGL
MOTA	119 0	GLU	15	10.107	53.492 139.757	1.00 19.72	HIGL
MOTA	120 N	GĽŰ	16	8.740	53.196 137.992	1.00 19.13	HIGL
MOTA	121 CA	GLU	16	7.562	53.084 138.839	1.00 19.39	HIGL
MOTA MOTA	122 CB 123 CG	GLU GLU	16 16	6.289 5.945	52.932 137.996 54.180 137.193	1.00 18.72 1.00 19.94	HIGL HIGL
ATOM	124 CD	GLU	16	4.840	53.959 136.159	1.00 13.34	HIGL
MOTA	125 OE1	GLU	16	4.817	52.881 135.521	1.00 22.23	HIGL
ATOM	126 OE2	GLU	16	4.003	54.874 135.966	1.00 21.65	HIGL
MOTA MOTA	127 C	GLU	16 16	7.759	51.885 139.761	1.00 19.47	HIGL
ATOM	128 O 129 N	GLU ARG	16 17	7.547 8.190	51.989 140.969 50.756 139.202	1.00 19.63 1.00 19.74	HIGL HIGL
				F= #	<b>A</b> = <b>1</b>		

Fig. 2 cont.

					U/ 1 / <del>- 1</del>		
ATOM	130 CA	ARG	17	8.416	49.562 140.014	1.00 20.25	HIGL
MOTA	131 CB	ARG	17	8.911	48.392 139.164	1.00 21.03	HIGL
ATOM	132 CG	ARG	17	7.873	47.765 138.257	1.00 23.68	HIGL
	132 CG		17	8.178	46.286 138.053	1.00 27.08	HIGL
MOTA		ARG				1.00 31.03	
ATOM	134 NE	ARG	17	7.410	45.701 136.956		HIGL
ATOM	135 CZ	ARG	17	7.660	45.919 135.664	1.00 32.87	HIGL
ATOM	136 NH1	ARG	17	8.666	46.709 135.299	1.00 32.97	HIGL
ATOM	137 NH2	ARG	17	6.902	45.352 134.731	1.00 33.75	HIGL
MOTA	. 138 C	ARG	17	9.445	49.840 141.104	1.00 19.92	HIGL
ATOM	139 0	ARG	17	9.443	49.198 142.151	1.00 20.42	HIGL
					50.801 140.850	1.00 19.29	HIGL
MOTA	140 N	ALA	18	10.325			
ATOM	141 CA	ALA	18	11.357	51.153 141.811	1.00 17.90	HIGL
ATOM	142 CB	ALA	18	12.584	51.698 141.086	1.00 17.12	HIGL
MOTA	143 C	ALA	18	10.846	52.168 142.830	1.00 17.59	$\mathtt{HIGL}$
ATOM	144 O	ALA	18	11.611	52.653 143.669	1.00 16.93	HIGL
ATOM	145 N	GLY	19	9.557	52.494 142.745	1.00 16.98	HIGL
ATOM	146 CA	GLY	19	8.963	53.424 143.687	1.00 16.15	HIGL
				8.935	54.890 143.298	1.00 16.93	HIGL
ATOM	147 C	GLY	19				
ATOM	148 O	GLY	19	8.543	55.734 144.104	1.00 17.33	HIGL
ATOM	149 N	VAL	20	9.333	55.209 142.072	1.00 17.17	HIGL
MOTA	150 CA	VAL	20	9.336	56.598 141.626	1.00 17.58	$\mathtt{HIGL}$
ATOM	151 CB	VAL	20	10.148	56.764 140.330	1.00 17.22	${\tt HIGL}$
ATOM	152 CG1	VAL	20	10.013	58.190 139.814	1.00 16.00	HIGL
ATOM	153 CG2	VAL	20	11.609	56.419 140.584	1.00 17.68	HIGL
	154 C			7.945	57.167 141.370	1.00 17.79	HIGL
ATOM		VAL	20				
ATOM	155 O	VAL	20	7.084	56.490 140.826	1.00 18.75	HIGL
MOTA	156 N	ARG	21	7.740	58.420 141.760	1.00 17.99	HIGL
MOTA	157 CA	ARG	21	6.470	59.106 141.537	1.00 18.92	HIGL
ATOM	. 158 CB	ARG	21	5.775	59.399 142.862	1.00 19.66	${\tt HIGL}$
ATOM	159 CG	ARG	21	5.367	58.155 143.617	1.00 20.84	HIGL
ATOM	160 CD	ARG	21	4.245	57.425 142.917	1.00 21.60	HIGL
	161 NE	ARG	21	3.389	56,783 143.906	1.00 23.75	HIGL
ATOM						1.00 23.73	HIGL
MOTA	162 CZ	ARG	21	3.734	55.707 144.598		
ATOM	163 NH1	ARG	21	4.920	55.148 144.389	1.00 25.67	HIGL
MOTA	164 NH2	ARG	21	2.911	55.215 145.516	1.00 22.10	HIGL
ATOM	165 C	ARG	21	6.749	60.412 140.809	1.00 18.45	HIGL
ATOM	166 O	ARG	21	7.598	61.198 141.231	1.00 18.88	HIGL
ATOM	167 N	TYR	22	6.032	60.640 139.717	1.00 17.66	HIGL
ATOM	168 CA	TYR	22	6.221	61.846 138.920	1.00 16.70	HIGL
MOTA	169 CB	TYR	22	6.236	61.480 137.438	1.00 15.81	HIGL
				7.402		1.00 16.16	HIGL
ATOM	170 CG	TYR	22		60.608 137.038		
MOTA	171 CD1	TYR	22	8.706	61.124 136.998	1.00 14.69	HIGL
ATOM	172 CE1	TYR	22	9.790	60.322 136.647	1.00 14.60	HIGL
ATOM	173 CD2	TYR	22	7.211	59.260 136.715	1.00 15.58	HIGL
MOTA	174 CE2	TYR	22	8.294	58.442 136.361	1.00 16.20	HIGL
ATOM	175 CZ	TYR	22 .	9.582	58.980 136.330	1.00 15.43	HIGL
MOTA	176 OH	TYR	22	10.648	58.178 135.994	1.00 12.55	HIGL
MOTA	177 C	TYR	22	5.156	62.903 139.166	1.00 17.06	HIGL
	-						
ATOM	178 O	TYR	22	4.008	62.591 139.482	1.00 17.73	HIGL
MOTA	179 ห	LYS	23	5.545	64.160 139.011	1.00 17.11	HIGL
ATOM	180 CA	LYS	23	4.631	65.279 139.191	1.00 17.49	HIGL
MOTA	181 CB	LYS	23	4.813	65.913 140.575	1.00 18.19	HIGL
MOTA	182 CG	LYS	23	4.800	64.938 141.748	1.00 19.57	HIGL
ATOM	183 CD	LYS	23	6.141	64.239 141.933	1.00 18.82	HIGL
	184 CE	LYS	23	6.061	63.255 143.085	1.00 18.77	HIGL
ATOM							HIGL
ATOM	185 NZ	LYS	23	7.366	62.602 143.352	1.00 19.04	HIGL
ATOM	186 C	LYS	23	4.975	66.318 138.137	1.00 17.45	
MOTA	187 O	LYS	23	6.098	66.342 137.640	1.00 17.10	HIGL
MOTA	188 N	ASN	24	4.021	67.171 137.786	1.00 17.71	HIGL
ATOM	189 CA	ASN	24	4.315	68,221 136.823	1.00 17.61	HIGL
ATOM	190 CB	ASN	24	3.029	68.792 136.210	1.00 17.78	HIGL
ATOM	191 CG	ASN	24	1.986	69.174 137.252	1.00 17.86	HIGL
					69.585 138.368	1.00 17.00	HIGL
ATOM	192 OD1	ASN	24	2.314			HIGL
MOTA	193 ND2	ASN	24	0.717	69.061 136.876	1.00 17.05	
ATOM	194 C	ASN	24	5.081	69.294 137.597	1.00 17.97	HIGL
					_		

Fig. 2 cont.

ATOM	195 O	ASN	24	5.481	69.060 138.739	1.00 16.84	HIGL
MOTA	196 N	VAL	25	5.285	70.462 136.994	1.00 19.12	${ t HIGL}$
					71.537 137.660	1.00 20.42	HIGL
ATOM	197 CA	VAL	25	6.033			
ATOM	198 CB	VAL	25	6.164	72.813 136.789	1.00 20.47	HIGL
	199 CG1	VAL	25	7.591	73.345 136.856	1.00 18.59	HIGL
MOTA							
ATOM	200 CG2	VAL	25	5.749	72.534 135.377	1.00 21.79	HIGL
MOTA	201 C	VAL	25	5.399	72.009 138.957	1.00 20.49	$\mathtt{HIGL}$
					72.577 139.812	1.00 19.69	
ATOM	202 O	VAL	25	6.071			
ATOM	203 N	ASN	26	4.101	71.782 139.094	1.00 21.96	$\mathtt{HIGL}$
ATOM	204 CA	ASN	26	3.375	72.242 140.271	1.00 22.88	HIGL
ATOM	205 CB	ASN	26	1.979	72.686 139.841	1.00 23.37	HIGL
ATOM	206 CG	ASN	26	2.026	73.861 138.879	1.00 24.96	$\mathtt{HIGL}$
			26	1.188	73.986 137.980	1.00 26.06	HIGL
ATOM	207 OD1	ASN					
MOTA	208 ND2	ASN	26	3.009	74.739 139.071	1.00 24.54	HIGL
ATOM	209 C	ASN	26	3.295	71.249 141.418	1.00 22.79	HIGL
					71.529 142.441	1.00 23.56	HIGL
MOTA	210 O	ASN	26	2,669			
ATOM	211 N	GLY	27	3.933	70.095 141.250	1.00 22.15	HIGL
ATOM	212. CA	GLY	27	3.932	69.094 142.299	1.00 20.67	HIGL
MOTA	213 C	GLY	27	2.743	68.157 142.290	1.00 19.93	HIGL
ATOM	214 0	GLY	27	2.574	67 <i>.</i> 357 143.214	1.00 20.18	HIGL
ATOM	215 N	GLN	28.	1.912	68.247 141.258	1.00 19.35	HIGL
ATOM	216 CA	GLN	28	0.748	67.376 141.164	1.00 19.04	HIGL
ATOM	217 CB	GLN	28	-0.314	68.025 140.274	1.00 19.46	HIGL
	218 CG	GLN	28	-1.579	67.207 140.102	1.00 19.85	HIGL
ATOM							
ATOM	219 CD	GLN	28	-2.666	67.970 139.363	1.00 21.15	HIGL
ATOM	220 OE1	GLN	28 ·	-2.425	68.547 138.299	1.00 21.73	· HIGL
						1.00 20.85	HIGL
ATOM	221 NE2	GLN	28	-3.871	67.971 139.921		
ATOM	222 C	GLN	28	1,164	66.009 140.607	1.00 18.84	HIGL
MOTA	223 O	GLN	28	1.602	65.901 139.464	1.00 18.45	HIGL
						1.00 18.66	HIGL
ATOM	224 N	GLU	29	1.038	64.973 141.432		
MOTA	225 CA	GLU	29	1.402	63.619 141.042	1.00 18.76	HIGL
ATOM	226 CB	GLU	29	1.487	62.730 142.287	1.00 18.41	HIGL
ATOM	227 CG	GLU	29	1.966	61.316 141.998	1.00 19.70	HIGL
ATOM	228 CD	GLU	29	2.223	60.504 143.252	1.00 21.17	HIGL
ATOM	229 OE1	GLU	29	2.828	61.042 144.204	1.00 22.90	HIGL
MOTA	230 OE2	GLU	29	1.836	59.318 143.285	1.00 21.00	HIGL
ATOM	231 C	GIJU	29	0.412	63.005 140.045	1.00 18.74	HIGL
ATOM	232 0	GLU	29	-0.793	63.133 140.205	1.00 20.35	HIGL
ATOM	233 N	LYS	30	0.929	62.357 139.007	1.00 18.03	HIGL
ATOM	234 CA	LYS	30	0.096	61.696 137.997	1.00 18.21	HIGL
ATOM	235 CB	LYS	30	-0.563	62.702 137.038	1.00 18.37	HIGL
ATOM	236 CG	LYS	30	-0.511	64.151 137.467	1.00 19.45	HIGL
MOTA	237 CD	LYS	30	-0.017	65.012 136.323	1.00 19.01	HIGL
					65.659 135.558	1.00 19.86	HIGL
ATOM	238 CE	LYS	30	-1.150			
ATOM	239 NZ	LYS	30	-1.471	67.014 136.095	1.00 19.22	HIGL
ATOM	240 C	LYS	30	0.999	60.777 137.179	1.00 17.33	HIGL
				2.227	60.837 137.297	1.00 18.02	HIGL
ATOM	241 0	LYS	30				
MOTA	242 N	PRO	31	0.404	59.905 136.353	1.00 16.17	HIGL
ATOM	243 CD	PRO	31	-1.032	59.580 136.274	1.00 16.56	HIGL
					58.991 135.525	1.00 15.20	HIGL
MOTA	244 CA	PRO	31	1.201			
ATOM	245 CB	PRO	31	0.147	58.122 134.854	1.00 15.51	HIGL
ATOM	246 CG	PRO	31	-1.001	58.135 135.843	1.00 16.29	HIGL
MOTA	247 C	PRO	31	1.992	59.830 134.521	1.00 15.68	HIGL
ATOM	248 O	PRO	31	1,455	60.782 133.943	1.00 16.00	HIGL
ATOM	249 N	LEU	32	3.258	59.478 134.313	1.00 14.62	HIGL
ATOM	250 CA	LEU	32	4.139	60.224 133.416	1.00 13.57	HIGL
MOTA	251 CB	LEU	32	5,433	59.437 133.198	1.00 12.66	${\tt HIGL}$
ATOM	252 CG	LEU	32	6.592	60.142 132.490	1.00 12.44	HIGL
ATOM	253 CD1	LEU	32	6.934	61,428 133.209	1.00 11.76	HIGL
ATOM	254 CD2	LEU	32	7.805	59,218 132.455	1.00 12.43	HIGL
							HIGL
ATOM	255 C	LEU	32	3.546	60.628 132.062	1.00 13.85	
ATOM	256 O	LEU	32	3.684	61.781 131.641	1.00 13.20	HIGL
ATOM	257 N	GLU	33	2.881	59,698 131.379	1.00 14.00	HIGL
							HIGL
ATOM	258 CA	GLU	33		60.020 130.073	1.00 14.95	
MOTA	259 CB	GLU	33	1.486	58.847 129.510	1.00 15.36	$\mathtt{HIGL}$

Fig. 2 cont.

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ATOM	260 CG	GLU	33	0.259	58.440 130.324	1.00 16.87	HIGL
			33		57.350 131.339	1.00 18.43	
ATOM	261 CD	GLU		0.560			HIGL
ATOM	262 OE1	GLU	33	1.586	57.459 132.049	1.00 19.77	HIGL
		GLU	33	-0.234	56.387 131.433	1.00 18.45	HIGL
ATOM	263 OE2						
ATOM	264 C	GLU	33	1.476	61.300 130.102	1.00 15.90	HIGL
ATOM	265 O	GLU	33	1.429	62.032 129.113	1.00 17.16	HIGL
ATOM	266 N	TYR	34	0.824	61.584 131.228	1.00 16.05	HIGL
				0.005	62.787 131.325	1.00 15.44	HIGL
MOTA	267 CA	TYR	34				
ATOM	268 CB	TYR	34	-1.104	62.593 132.358	1.00 16.32	HIGL
			-				HIGL
ATOM	269 CG	TYR	34	-2.087	61.551 131.901	1.00 16.99	
MOTA	270 CD1	TYR	34	-2.063	60.257 132.426	1.00 17.20	$\mathtt{HIGL}$
MOTA	271 CE1	TYR	34	-2.915	59.267 131.937	1.00 17.14	HIGL
ATOM	272 CD2	TYR	34	-2.992	61.832 130.875	1.00 17.08	HIGL
	273 CE2				60.851 130.378	1.00 17.17	HIGL
ATOM		TYR	34	-3.845			
ATOM	274 CZ	TYR	34	-3.801	59.572 130.913	1.00 17.87	HIGL
ATOM	275 OH	TYR	34	-4.647	58.603 130.425	1.00 19.84	HIGL
ATOM	276 C	TYR	34	0.828	64.030 131 <i>.</i> 617	1.00 14.61	HIGL
ATOM	277 O	TYR	34	0.512	65.115 131.126	1.00 13.80	HIGL
MOTA	278 N	ILE	35	1.889	63.880 132.399	1.00 14.26	${ t HIGL}$
ATOM	279 CA	ILE	35 -	2.763	65.014 132.672	1.00 14.92	HIGL
ATOM	280 CB	ILE	35	3.865	64.662 133.679	1.00 15.08	HIGL
ATOM	281 CG2	ILE	35	4.882	65.794 133.753	1.00 14.72	HIGL
ATOM	282 CG1	ILE	35	3.243	64.398 135.051	1.00 15.03	$\mathtt{HIGL}$
MOTA	283 CD1	ILE	35 ·	4.219	63.877 136.067	1.00 15.01	HIGL
ATOM	284 C	ILE	35	3.424	65.404 131.352	1.00 14.91	${\tt HIGL}$
MOTA	285 O	ILE	35	3.656	66.584 131.092	1.00 15.44	HIGL
							•
MOTA	286 N	LEU	36	3.715	64.403 130.518	1.00 14.83	$\mathtt{HIGL}$
ATOM	287 CA	LEU	36	4.332	64.649 129.215	1.00 14.44	HIGL
ATOM	288 CB			4.765	63.340 128.557		HIGL
		LEU	36			1.00 14.34	
ATOM	289 CG	LEU	36	5.806	62.491 129.280	1.00 15.12	HIGL
ATOM	290 CD1	LEU	36	6.153	61.306 128.385	1.00 15.81	HIGL
ATOM	291 CD2	LEU	36	7.050	63.320 129.595	1.00 13.46	HIGL
ATOM	292 C	LEU	36	3.385	65.375 128.267	1.00 14.40	HIGL
ATOM	293 O	LEU	[.] 36	3.761	66.376 127.659	1.00 13.88	HIGL
ATOM	294 N	ALA	37	2.162	64.864 128.131	1.00 14.45	HIGL
ATOM	295 CA	ALA	37	1.173	65.482 127.247	1.00 15.05	HIGL
MOTA	296 CB	ALA	37	-0.121	64.677 127.269	1.00 14.89	HIGL
ATOM	297 C	ALA	37	0.918	66.915 127.711	1.00 15.47	${ t HIGL}$
MOTA	298 O	ALA	37	0.757	67.832 126.907	1.00 14.62	${\tt HIGL}$
	299 N						
MOTA		GLÜ	38	0.910	67.081 129.028	1.00 16.62	${\tt HIGL}$
ATOM	300 CA	GLU	38	0.693	68.362 129.689	1.00 17.33	HIGL
ATOM	301 CB	GLU	38	0.784	68.145 131.200	1.00 19.24	HIGL
ATOM	302 CG	GĽU	38	0.365	69.311 132.054	1.00 21.29	HIGL
ATOM	303 CD	GLU	38	0.550	69.028 133.529	1.00 22.16	HIGL
ATOM	304 OE1	GLU	38	0.222	67.905 133.972	1.00 21.31	HIGL
ATOM	305 OE2	GLU	38	1.018	69.939 134.244	1.00 23.91	HIGL
ATOM	306 C	GLU	38	1.727	69.402 129.262	1.00 16.88	HIGL
MOTA	307 O	GLU	38	1.441	70.597 129.205	1.00 16.84	HIGL
						1.00 16.61	
MOTA	308 N	ASN	39	2.934	68.942 128.960	1.00 10.01	$\mathtt{HIGL}$
MOTA	309 CA	ASN	39	4.010	69.841 128.569	1.00 16.17	HIGL
ATOM	310 CB	ASN	39	5.311	69.379 129.218	1.00 16.22	HIGL
MOTA	311 CG	ASN	39	5.441	69.846 130.650	1.00 16.62	HIGL
MOTA	312 OD1	ASN	39	5.928	70.948 130.907	1.00 16.26	HIGL
ATOM	313 ND2	ASN	39	4.991	69.017 131.594	1.00 15.54	HIGL
ATOM	314 C	ASN	39	4.218	70.024 127.067	1.00 16.04	HIGL
MOTA	315 O	ASN	39	5.226	70.597 126.649	1.00 16.85	HIGL
ATOM	316 N	GLY	40	3.279	69.535 126.259	1.00 15.42	HIGL
ATOM	317 CA	GLY	40	3.392	69.694 124.821	1.00 14.77	HIGL
ATOM	318 C	GLY	40	3.895	68.494 124.037	1.00 15.22	HIGL
ATOM	319 O	GLY	40	3.890	68.517 122.810	1.00 15.07	$\mathtt{HIGL}$
ATOM	320 N	VAL	41	4.342	67.451 124.725	1.00 15.28	HIGL
ATOM	321 CA	VAL	41	4.822		1.00 15.01	HIGL
					66.257 124.038		
ATOM	322 CB	VAL	41	5.357	65.212 125.047	1.00 15.77	HIGL
ATOM	323 CG1	VAL	41	5.682	63.896 124.328	1.00 14.74	HIGL
ATOM	324 CG2	VAL	41	6.596	65.760 125.751	1.00 15.28	HIGL

Fig. 2 cont.

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				51	1/174		
7.004	705 6	UAT.	41	3.668		1.00 14.29	HIGL
ATOM	325 C	VAL VAL	41	2.560	65.558 123.776	1.00 14.34	HIGL
ATOM	326 O 327 N	ASN	42	3.913	65.230 122.017	1.00 14.20	HIGL
MOTA MOTA	327 N 328 CA	ASN	42	2.846	64.611 121.217	1:00 14.11	HIGL
ATOM	329 CB	ASN	42	2.451	65.488 120.008	1.00 13.09	HIGL
ATOM	330 CG	ASN	42	3.588	65.683 119.003	1.00 15.29	HIGL
ATOM	331 OD1	ASN	42	4.632	65.030 119.077	1.00 14.89	HIGL
MOTA	332 ND2	ASN	42	3.376	66.587 118.044	1.00 13.72	HIGL
ATOM	333 C	ASN	42	3.220	63.215 120.734	1.00 13.63	HIGL
ATOM	334 0	ASN	42	2.523	62.628 119.907	1.00 13.90	HIGL
ATOM	335 N	MET	43	4.319	62.683 121.259	1.00 13.09	HIGL
ATOM	336 CA	MET	43	4.776	61.355 120.865	1.00 12.43	HIGL HIGL
MOTA	337 CB	MET	43	5.290	61.373 119.421	1.00 12.54 1.00 13.16	HIGL
ATOM	338 CG	MET	43	5.833	60.029 118.943	1.00 15.10	HIGL
ATOM	339 SD	MET	43	6.153	59.988 117.164 60.024 116.523	1.00 14.86	HIGL
MOTA	340 CE	MET	43	4.461	60.820 121.774	1.00 11.00	HIGL
ATOM	341 C .	MET	43	5.870 6.730	61.563 122.229	1.00 9.98	HIGL
ATOM	342 O	MET	43	5.824	59.522 122.041	1.00 10.40	HIGL
MOTA	343 N	VAL	`44 44	6.837	58.900 122.872	1.00 10.47	HIGL
ATOM	344 CA 345 CB	VAL VAL	44	6,218	58.213 124.113	1.00 10.16	HIGL
ATOM ATOM	345 CB 346 CG1	VAL	44	5.663	59.259 125.057	1.00 10.97	HIGL
ATOM	347 CG2	VAL	44	5.120	57.251 123.696	1.00 10.36	HIGL
ATOM	348 C	VAL	44	7.607	57.868 122.051	1.00 10.89	HIGL
ATOM	349 0	VAL	44	7.060	57.241 121.140	1.00 9.61	HIGL
ATOM	350 N	ARG	45	8.889	57.721 122.368	1.00 11.52	HIGL
ATOM	351 CA	ARG	45 ·	9.758	56.765 121.696	1.00 12.77	HIGL
ATOM	352 CB	ARG.	45 .	11.085	57.442 121.351	1.00 14.01	HIGL HIGL
MOTA	353 CG	ARG	45	12.129	56.570 120.667	1.00 15.59 1.00 16.97	HIGL
MOTA	354 CD	ARG	45	13.326	57.430 120.305 56.694 119.679	1.00 10.37	HIGL
ATOM	355 NE	ARG	45	14.418	56.254 120.320	1.00 17.82	HIGL
MOTA	356 CZ	ARG	45	15.496 15.642	56.466 121.620	1.00 17.90	HIGL
ATOM	357 NH1 358 NH2	ARG ARG	45 45	16.439	55.610 119.653	1.00 18.55	HIGL
ATOM ATOM	359 C	ARG	45	9.970	55.628 122.687	1.00 13.22	HIGL
ATOM	360 O	ARG	45	10.244	55.870 123.859	1.00 13.66	HIGL
ATOM	361 N	GLN	46	9.821	54.390 122.232	1.00 13.78	HIGL
ATOM	362 CA	GLN	46	9.996	53.243 123.118	1.00 14.54	HIGL
ATOM	363 CB	GLN	46	8.639	52.573 123.394	1.00 15.20	HIGL
MOTA	364 CG	GLN	46	7.582	53.492 124.043	1.00 16.94	HIGL HIGL
ATOM	365 CD	GLN	46	6.298	52.748 124.403	1.00 18.02 1.00 17.27	HIGL
ATOM	366 OE1	GLN	46	5.361	53.328 124.944 51.454 124.097	1.00 17.27	HIGL .
ATOM	367 NE2	GLN	46	6.257 10.960	52.228 122.512	1.00 14.27	HIGL
MOTA	368 C	GLN	46 46	10.808	51.829 121.360	1.00 15.12	HIGL
ATOM ATOM	369 O 370 N	GLN ARG	47	11.962	51.821 123.280	1.00 14.18	HIGL
ATOM	371 CA	ARG	47	12.923	50.847 122.787	1.00 14.34	HIGL
MOTA	372 CB	ARG	47	14.264	51,008 123.510	1.00 14.68	HIGL
ATOM	373 CG	ARG	47	14.172	51.059 125.026	1.00 14.19	HIGL
ATOM	374 CD	ARG	47	15.555	50.900 125.661	1.00 14.01	HIGL
MOTA	375 NE	ARG	47	15.530	51.133 127.101	1.00 13.64	HIGL
ATOM	376 CZ	ARG	47	15.463	52.341 127.651	1.00 13.65	HIGL
MOTA	377 NH1	ARG	47	15.422	53.415 126.872	1.00 12.61	HIGL
ATOM	378 NH2	ARG	47	15.436		1.00 12.29 1.00 14.38	HIGL
ATOM	379 C	ARG	47	12.375		1.00 14.36	HIGL
MOTA	380 0	ARG	47	11.742 12.616		1.00 14.20	HIGL
MOTA	381 N	VAL	48	12.136		1.00 14.15	HIGL
ATOM	382 CA 383 CB	VAL VAL	48 48	11,108		1.00 14.30	HIGL
ATOM ATOM	384 CG1		48	10.497		1.00 12.51	HIGL
MOTA	385 CG2		48	10.044		1.00 14.44	HIGL
MOTA	386 C	VAL	48	13.266	46.185 121.901	1.00 15.87	HIGL
ATOM	387 O	VAL	48	13.987	46.200 120.903	1.00 16.88	HIGL
MOTA	388 N	TRP	49	13.420	45.319 122.901	1.00 16.25	HIGL
ATOM	389 CA	TRP	49	14.449	44.283 122.881	1.00 16.07	HIGL

Fig. 2 cont.

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EΩ	14	71
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				V	<i></i>		
MOTA	390 CI	B TRE	49	15.243	44.280 124.194	1.00 15.19	HIGL
				16.039	45.533 124.422	1.00 15.37	HIGL
ATOM	391 C						
ATOM	392 C	D2 TRE	49	16.745	45.898 125.613	1.00 15.05	HIGL
MOTA	393 C	E2 TRE	49	17.359	47.146 125.370	1.00 14.69	HIGL
				16.922	45.290 126.864		HIGL
ATOM	394 C				-	_	
MOTA	395 C	D1 TRE	49	16.247	46.550 123.529	1.00 15.47	HIGL
ATOM	396 N		49	17.037	47.521 124.093	1,00 14.49	HIGL
MOTA	397 C	Z2 TRE		18.138	47.798 126.332		HIGL
ATOM	398 C	Z3 TRE	49	17.696	45.939 127.819	1.00 14.43	HIGL
	399 C			18.294	47.179 127.547		HIGL '
MOTA							
MOTA	400 C	TRE	9 49	13.793	42.924 122.665	1.00 16.51	$\mathtt{HIGL}$
MOTA	401 O	TRE	49	12.657	42.695 123.100	1.00 16.05	HIGL
MOTA	402 N			14.517	42.031 121.990		HIGL
MOTA	403 C	A VAI	50	14.031	40.690 121.675	1.00 17.15	${ t HIGL}$
ATOM	404 C			15.039	39.953 120.754	1.00 17.71	HIGL
			_				
MOTA	405 C	G1 VAI	50	14.449	38.639 120.260		HIGL
ATOM	406 C	G2 VAI	50	15.402	40.841 119.571	1.00 17.23	HIGL
ATOM	407 C			13.763	39.843 122.923		HIGL
MOTA	408 O	VAI	50	12.617	39.724 123.362		HIGL
ATOM	409 N	ASN	N 51	14.812	39.258 123.495	1.00 18.58	HIGL
				14.660	38.430 124.690		HIGL
ATOM	410 C						
MOTA	411 C	B ASI	v 51	15.126	37.010 124.410	1.00 21.64	HIGL
ATOM	412 C	G ASI	v 51	14.602	36.480 123.093	1.00 24.95	HIGL
					36.364 122.892		HIGL
ATOM	413 O						
ATOM	414 N	D2 ASI	v 51	15.517	36.156 122.180	1.00 25.56	HIGL
ATOM	415 C	ASI	v 51	15.443	38.978 125.875	1.00 18.38	HIGL
							HIGL
· MOTA	416 O			16.417	38.368 126.319		
ATOM	417 N	PRO	52	15.032	40.144 126.401	1.00 17.80	$\mathtt{HIGL}$
MOTA	418 C	D PRO	52	13.867	40.972 126.053		$\mathtt{HIGL}$
						-	
ATOM	419 C			15.747	40.712 127.543		HIGL
MOTA	420 C	B PRO	52	14.949	41.971 127.861	1.00 16.91	HIGL
ATOM	421 C			13.579	41.650 127.364	1.00 17.23	HIGL
MOTA	422 C	: PRO		15.776	39.716 128.688		HIGL
ATOM	423 O	PRO	52	14.828	38.954 128.891	1.00 17.99	HIGL
ATOM	424 N			16.877	39,723 129,428		HIGL
ATOM	425 C	A TR	P 53	17.068	38.801 130.536		HIGL
ATOM	426 C	B TRI	P 53	18.448	39.013 131.156	1.00 18.06	HIGL
ATOM	427 C			18.543	40.298 131.917		HIGL
MOTA	428 C	D2 TR	P · 53	18.389	40.459 133.328	3 1.00 18.71	HIGL
ATOM	429 C	E2 TR	P 53	18.452	41.844 133.600	1.00 17.92	HIGL
	430 C			18.198	39.565 134.390		HIGL
MOTA							
ATOM	431 C	D1 TR	P 53	18.698	41.553 131.404	1.00 18.32	HIGL
MOTA	432 N	EI TR	P 53	18.642	42.489 132.409	1.00 17.61	HIGL
ATOM	433 C			18.331	42.357 134.888		HIGL
ATOM	434 C	23 TR	P 53	18.077	40.074 135.674	1.00 19.45	HIGL
MOTA	435 C	H2 TR	P 53	18.143	41.460 135.912	2 1.00 19.83	HIGL
ATOM	436 C			16.017	38.919 131.631		HIGL
ATOM	437 O	TR:	P 53	15.726	37.944 132.324	1.00 18.33	HIGL
MOTA	438 N	I AS	P 54	15.447	40.106 131.793	3 1.00 17.42	HIGL
				14.455	40.307 132.845		HIGL
ATOM	439 C						
ATOM	440 C	B AS	P 54	14.976	41.352 133.830		HIGL
ATOM	441 C	G AS	P 54	15.139	42.705 133.189	9 1.00 17.98	HIGL
					42.779 131.938		HIGL
MOTA	442 C			15.083			
ATOM	443 C	D2 AS	P 54	15.325	43.690 133.927	7 1.00 17.75	HIGL
ATOM	444 C	: AS	P 54	13.080	40.718 132.320	1.00 16.46	HIGL
							HIGL
ATOM	445 C			12.196	41.080 133.094		
ATOM	446 N	I GL	Y 55	12.907	40.666 131.00	3 1.00 16.49	HIGL
ATOM	447 C			11.629	41.019 130.40	5 1.00 15.10	HIGL
MOTA	448 C			11.396	42.494 130.120		HIGL
ATOM	449 C	) GL	Y 55	10.461	42.844 129.40	L 1.00 14.82	HIGL
ATOM	450 N			12.225	43.375 130.66		HIGL
ATOM	451 C			12.010	44.792 130.418		HIGL
ATOM	452 C	B AS	N 56	12.784	45.649 131.41	7 1.00 14.38	HIGL
ATOM	453 C			12.130	45.660 132.78		HIGL
ATOM	454 C	DI AS	N 56	10.901	45.606 132.90	2 1.00 15.70	HIGL

Fig. 2 cont.

				53	3/174		
ATOM	455 ND2	ASN	56	12.941	45.743 133.826	1.00 16.95	HIGL
ATOM	456 C	ASN	56	12.341		1.00 13.31 1.00 12.12	HIGL HIGL
ATOM	457 O	ASN	56	13.366		1.00 12.12	HIGL
ATOM	458 N	TYR	57 . 57	11.439 11.558		1.00 13.09	HIGL
ATOM ATOM	459 CA 460 CB	TYR TYR	57 57	12.968		1.00 12.20	HIGL
ATOM	461 CG	TYR	57	13.466	47.989 127.865	1.00 11.14	HIGL
ATOM	462 CD1	TYR	57	12.666	49.030 128.330	1.00 10.28	HIGL HIGL
ATOM	463 CE1	TYR	57	13.095	49.859 129.353 47.808 128.450	1.00 9.79 1.00 10.12	HIGL
ATOM	464 CD2	TYR	57 57	14.716 15.152	48.630 129.471	1.00 9.28	HIGL
ATOM ATOM	465 CE2 466 CZ	TYR TYR	57	14.333	49.654 129.922	1.00 9.42	HIGL
MOTA	467 OH	TYR	57	14.737	50.450 130.973	1.00 10.17	HIGL
ATOM	468 C	TYR	57	11.214	45.426 126.052	1.00 13.71 1.00 13.96	HIGL HIGL
MOTA	469 0	TYR	57	11.460 10.657	45.591 124.854 44.313 126.515	1.00 13.75	HIGL
ATOM	470 N 471 CA	asn asn	58 58	10.276	43.298 125.553	1.00 14.27	HIGL
ATOM ATOM	472 CB	ASN	58	10.325	41.874 126.147	1.00 12.09	HIGL
ATOM	473 CG	ASN	58	9.216	41.576 127.140	1.00 9.87	HIGL HIGL
MOTA	474 OD1	ASN	58	8.278	42.353 127.323	1.00 11.38 1.00 5.89	HIGL
ATOM	475 ND2	ASN	58 58	9.316 8.892	40.416 127.777 43.669 125.039	1.00 15.29	HIGL
ATOM ATOM	476 C 477 O	ASN ASN	58	8.301	44.651 125.490	1.00 14.81	HIGL
ATOM	478 N	LEU	59	8.389	42.901 124.085	1.00 17.30	HIGL
ATOM	479 CA	LEU	59	7.096	43.188 123.482	1.00 19.48 1.00 21.08	HIGL HIGL
ATOM	480 CB	LEU	59	6.692 5.709	42.037 122.565 42.447 121.470	1.00 21.00	HIGL
ATOM	481 CG 482 CD1	LEU	59 59	6.296	43.624 120.673	1.00 23.05	HIGL
ATOM ATOM	483 CD2	LEU	59	5.436	41.247 120.561	1.00 23.47	HIGL
ATOM	484 C	LEU	59	5.970	43.488 124.471	1.00 19.90	HIGL HIGL
MOTA	485 O	LEU	59	5.367	44.557 124.415 42.555 125.372	1.00 21.04 1.00 20.10	HIGL
MOTA	486 N	ASP	60 60	5.683 4.619	42.756 126.348	1.00 20.50	HIGL
MOTA MOTA	487 CA 488 CB	ASP ASP	60	4.599	41.613 127.369	1.00 21.74	HIGL
ATOM	489 CG	ASP	60	4-436	40.250 126.720	1.00 23.55	HIGL
ATOM	490 OD1	ASP	60	3.553	40.100 125.844	1.00 23.00 1.00 24.89	HIGL HIGL
ATOM	491 OD2	ASP	60 60	5.190 4.810	39.324 127.094 44.078 127.078	1.00 20.77	HIGL
ATOM ATOM	492 C 493 O	ASP ASP	60	3.869	44.860 127.231	1.00 21.37	HIGL
ATOM	494 N	TYR	61	6.038	44.315 127.529	1.00 20.29	HIGL
ATOM	495 CA	TYR	61	6.393	45.533 128.241	1.00 19.19 1.00 19.77	$ ext{HIGL}$
MOTA	496 CB	TYR	61	7.896 8.400	45.526 128.574 46.776 129.274	1.00 19.20	HIGL
ATOM	497 CG 498 CD1	TYR TYR	61 61	8.572	47.975 128.580	1.00 19.12	HIGL
ATOM ATOM	499 CE1	TYR	61	8.998	49.132 129.229	1.00 19.60	HIGL
ATOM	500 CD2	TYR	61	8.675	46.766 130.638	1.00 19.18	HIGL HIGL
ATOM	501 CE2		61	9.101	47.916 131.297 49.096 130.589	1.00 20.13 1.00 20.45	HIGL
ATOM	502 CZ	TYR TYR	61 61	9.259 9.663	50.239 131.250	1.00 21.00	HIGL
ATOM ATOM	503 OH 504 C	TYR	61	6.059	46.767 127.414	1.00 19.25	HIGL
MOTA	505 0	TYR	61	5.506	47.738 127.930	1.00 19.40	HIGL HIGL
MOTA	506 N	ASN	62	6.390	46.733 126.129	1.00 19.00 1.00 19.77	HIGL
MOTA	507 CA	ASN	62 62	6.128 6.971	47.878 125.271 47.789 123.999	1.00 20.44	HIGL
ATOM ATOM	508 CB 509 CG	ASN ASN	62	8.403		1.00 21.08	HIGL
ATOM	510 OD1		62	8.685	49.415 124.376	1.00 21.94	HIGL
ATOM	511 ND2	ASN	62	9.315		1.00 20.37	HIGL HIGL
MOTA	512 C	ASN	62	4.664		1.00 19.75 1.00 20.46	HIGL
ATOM	513 O 514 N	ASN I LE	62 63	4.235 3.892			HIGL
MOTA MOTA	514 N 515 CA	ILE	63	2.472	47.073 124.717	1.00 20.26	HIGL
ATOM	516 CB	ILE	63	1.856	45.693 124.478	1.00 20.11	HIGL
ATOM	517 CG2		63	0.336	45.761 124.598	1.00 19.41 1.00 20.67	HIGL HIGL
ATOM	518 CG1 519 CD1		63 63	2.293 1.599			HIGL
ATOM	フェラ しひょ		55	255			

Fig. 2 cont.

				54	1/174		
a moss	520 C	ILE	63 ·	1.742	47.775 125.852	1.00 21.15	HIGL
ATOM ATOM	521 0	ILE	63	0.807	48.535 125.617	1.00 20.59	HIGL
ATOM	522 N	GLN	64 .	2.172	47.528 127.086	1.00 22.72	HIĢL
ATOM	523 CA	GLN	64	1.547	48.177 128.235	1.00 23.28	HIGL
ATOM	524 CB	GLN	64	2.117	47.626 129.544	1.00 24.62	HIGL
ATOM	525 CG	GLN	64	1.064	47.428 130.630	1.00 27.22	HIGL
ATOM .	526.CD	GLN	64	1.641	46.837 131.906	1.00 29.98	HIGL
ATOM	527 OE1	GLN	64 · ·	2.314	45.798 131.877	1.00 31.39	HIGL
ATOM	528 NE2	GLN	64	1.380	47.493 133.037	1.00 29.60	HIGL
ATOM	529 C	GLN	64	1.827	49.675 128.130	1.00 22.91	HIGL
ATOM	530 O	GLN	64	0.952	50.501 128.400	1.00 23.24	HIGL
ATOM	531 N	LEU	65	3.045	50.018 127.717	1.00 21.90	HIGL HIGL
ATOM . ;	532 CA .	LEU	65	3.436	51.415 127.559	1.00 21.80	HIGL
.ATOM	533 CB	LEU	65	4.925	51.524 127.241	1.00 21.78 1.00 22.02	HIGL
MOTA	534 CG	LEU	65	5.863	51.436 128.439	1.00 22.02	HIGL
MOTA	535 CD1	LEU	65	7.300	51.702 128.006	1.00 21.72	
MOTA	536 CD2	LEU	65	5.424	52.459 129.459	1.00 22.32	HIGL
ATOM .	537 C	LEU	65 .	2.650	52.104 126.458 53.191 126.651	1.00 20.27	HIGL
MOTA	538 0	LEU	65	2.107 2.604	51.467 125.297	1.00 21.88	HIGL
ATOM	539 N '	ALA'	66 .	1.884	52.017 124.157	1.00 22.71	HIGL
ATOM	540 CA	ALA	66 [·]	1.908	51.026 123.006	1.00 21.67	HIGL
ATOM	541 CB	ALA . ALA	66	0.447	52.340 124.546	1.00 22.91	HIGL
ATOM	. 542 C . 543 O	ALA	66∴	-0.013	53.471 124.395	1.00 23.72	HIGL
ATOM ATOM	. 543 O	ARG	67 ·	-0.256	51.340 125.059	1.00 23.00	HIGL
ATOM .	545 CA	ARG	67	-1.635	51.517 125.457	1.00 22.83	HIGL
ATOM	546 CB	ARG	67	-2.121	50.260 126.173	1.00 24.13	HIGL
ATOM	547 CG	ARG	67	-3.621	50.147 126.305	1.00 26.38	HIGL
ATOM	548 CD	ARG	67	-3.993	48.774 126.824	1.00 29.10	HIGL
ATOM	549 NE	ARG	67	-3.810	47.732 125.815	1.00 30.83	HIGL HIGL
ATOM	550 CZ	ARG	67	-3.501	46.469 126.098	1.00 32.31	HIGL
ATOM	551 NH1	ARG	67	-3.333	46.096 127.361	1.00 33.65 1.00 32.30	HIGL
MOTA	552 NH2	ARG	67	-3.369	45.576 125.126 52.749 126.351	1.00 32.30	HIGL
ATOM	553 C	ARG	67 63	-1.747 -2.627	53.587 126.158	1.00 22.49	HIGL
ATOM	554 O	ARG	67 68	-0.843	52.876 127.313	1.00 21.00	HIGL
ATOM	555 N 556 CA	ARG ARG	68	-0.860	54.031 128.207	1.00 20.10	HIGL
ATOM ATOM	557 CB	ARG	68	0.183	53.867 129.321	1.00 19.58	HIGL
ATOM	558 CG	ARG	68	-0.247	52.927 130.442	1.00 18.60	HIGL
ATOM	559 CD	ARG	68	0.858	52.723 131.475	1.00 17.98	HIGL
ATOM	560 NE	ARG	68	1.319	53.986 132.048	1.00 17.78	HIGL
ATOM	561 CZ	ARG	68	2.210	54.078 133.030	1.00 16.65	HIGL
ATOM	562 NH1	ARG	68	2.735	52.975 133.550	1.00 15.08	HIGL
ATOM	563 NH2	ARG	68	2.574	55.272 133.490	1.00 15.87 1.00 20.06	HIGL
ATOM	564 C	ARG	68	-0.588	55.322 127.441	1.00 19.99	HIGL
ATÓM	565 O	ARG	68	-1.287	56.312 127.613 55.306 126.597	1.00 20.75	HIGL
MOTA	566 N	ALA	69	0.437 0.800		1.00 21.00	HIGL
ATOM	567 CA	ALA	69	1.979		1.00 21.37	HIGL
ATOM	568 CB	ALA ALA	69 69	-0.379		1.00 21.40	HIGL
MOTA	569 C 570 O	ALA	69	-0.610			HIGL
ATOM ATOM	571 N	LYS	70	-1.114		1.00 21.23	HIGL
· ATOM	572 CA	LYS	70	-2.273		1.00 22.04	HIGL
ATOM	573 CB	LYS	70	-2.770	54.991 122.941	1.00 24.06	HIGL
ATOM	574 CG	LYS	70	-4.006	55.118 122.060	1.00 26.72	HIGL
ATOM	575 CD	LYS	70	-4.553			HIGL
ATOM	576 CE	LYS	70 .	-5.785			HIGL
ATOM	577 NZ	LYS	70	-6.349			HIGL
MOTA	578 C	LYS	70	-3.394	56.946 124.403	1.00 21.81	HIGL HIGL
ATOM	579 O	LYS	70	-4.034	57.901 123.958	1.00 21.40	HIGL
ATOM	580 N	ALA	71	-3.631	56.439 125.609	1.00 20.36	HIGL
MOTA	581 CA	ALA	71	-4.682			HIGL
ATOM	582 CB	ALA	71	-4.770			HIGL
MOTA	583 C	ALA	71 73	-4.432 -5.371			HIGL
ATOM	584 O	ALA	71		, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		

-5.371 59.259 126.862 Fig. 2 cont.

5	5/1	74
6	58.	881
2	60	276

						1.00 18.45	HIGL
ATOM .	585 N	ALA	72	-3.166	58.881 126.754	1.00 18.43	
	586 CA	ALA	72	-2.822	60.276 126.987	1.00 17.24	t HIGL
ATOM			. 72	-1.507	60.374 127.753	1.00 16.31	HIGL
ATOM	587 CB	ALA ·		-2.722	61.035 125.667	1.00 16.70	HIGL
MOTA	588 C	ALA	72 .			1.00 17.88	HIGL
ATOM	·589 O	ALA	72	-2.210	62.147 125.628		
ATOM	590 N	GLY	73	-3.200	60.421 124.589	1.00 15.95	HIGL
			73	-3.176	61.058 123.284	1.00 15.41	HIGL
ATOM	591 CA	GLY			61.236 122.647	1.00 16.92	HIGL
ATOM	592 C	GLY	73	1.809	01.236 122.047		HIGL
ATOM .	593°O	GLY	73	-1.638	62.056 121.739	1.00 16.80	
ATOM	594 N	LEU	74	-0.826	60.470 123.107	1.00 16.80	${ t HIGL}$
				0.516	60.577 122.554	1.00 16.41	HIGL
ATOM	595 CA	LEU	74		60.366 123.663	1.00 15.23	HIGL
ATOM	596 CB	LEU	74	1.545	60.366 123.663		HIGL
ATOM	597 CG	LEU	74	1.311	61.253 124.884	1.00 14.82	
ATOM	'598 CD1	LEU	74	2.265	60.875 125.994	1.00 13.72	HIGL
		•	-	1.486	62.706 124.492		HIGL
ATOM	599 CD2	LEU	74				HIGL
MOTA	600 C	LEU	74	0.762	59.577 121.424		HIGL
ATOM	601 O	LEU	74	0.319	58.430 121.482	1.00 16.67	
ATOM	602 N	GLY	75	1.470	60.027 120.392	1.00 18.17	HIGL
			.5 75	1.785	59.155 119.278		${\tt HIGL}$
ATOM	603 CA	GLY			58.153 119.695		HIGL
ATOM	604 C	GLY	75	2.846	38.133 119.092		HIGL
MOTA	605 O	GLY	75	3.486	58.299 120.748		
ATOM	606 N	LEU	76	3.058	57.147 118.858	1.00 17.36	HIGL
		LEU	76	4.014	56.103 119.163		${ t HIGL}$
MOTA	607 CA				54.777 119.306		HIGL
ATOM	608 CB	LEU	76	3.262	54.777 119.500		HIGL
MOTA	609 CG	LEU	76	4.075	53.527 119.631	1.00 17.06	
ATOM	610 CD1	LEU	· 76	4.742	53.691 120.997	1.00 16.56	HIGL
	611 CD2	LEU	76	3.161	52.318 119.620	1.00 15.85	$\mathtt{HIGL}$
ATOM				5.143	55.949 118.139		$\mathtt{HIGL}$
MOTA	612 C	LEU '	76		55.918 116.932		HIGL
ATOM	613 0	LEU	76	4.914			HIGL
ATOM	614 N	TYR	77	6.364	55.844 118.648		
ATOM	. 615 CA	TYR	· 77	7,560	55.664 117.835	1.00 15.08	HIGL
			77	8.420	56.938 117.927	1.00 14.34	HIGL
ATOM	616 CB	TYR			56.872 117.439		HIGL
ATOM	617 CG	TYR	77	9.866			HIGL
MOTA	618 CD1	TYR	77	10.428	55.695 116.92		
ATOM	619 CE1	TYR	77	11.774	55.644 116.552	2 1.00 14.56	HIGL
ATOM	620 CD2	TYR	77	10.693	57.994 117.54	7 1.00 15.32	$\mathtt{HIGL}$
				12.039	57.955 117.17		HIGL
ATOM	621 CE2	TYR	77		56.783 116.68		HIGL
ATOM	622 CZ	TYR	77	12.577			HIGL
ATOM	623 OH	TYR	77	13.920	56.753 116.36		
MOTA	624 C	TYR	77	8.261	54.436 118.44	0 1.00 15.55	HIGL
	625 0	TYR	77	8.853	54.507 119.53	0 1.00 15.30	$\mathtt{HIGL}$
ATOM				8.147	53.306 117.74		HIGL
ATOM	626 N	ILE	78.				HIGL
ATOM	627 CA	ILE	78	8.751	52.051 118.18		
ATOM	628 CB	ILE	78	7.970	50.824 117.63		HIGL
MOTA	629 CG2	ILE	78	8.742	49.534 117.93	0 1.00 14.89	$\mathtt{HIGL}$
	630 CG1	ILE	78	6.575	50.766 118.27	6 1.00 14.25	HIGL
MOTA							HIGL
MOTA	631 CD1	ILE	78	6.567	50.420 115.70	1 1.00 13.40	HIGL
MOTA	632 C	ILE	78	10.193	51.991 117.70		
ATOM	633 O	ILE	78	10.467	52.112 116.51	2 1.00 13.27	HIGL
	634 N	ASN	79	11.104	51.797 118.64	6 1.00 13.08	HIGL
MOTA				12.533			HIGL
MOTA	635 CA	ASN	79				HIGL
ATOM	636 CB	ASN	79	13.209	52.771 119.30		
MOTA	637 CG	ASN	79	14.714	52.607 119.39	3 1.00 12.44	HIGL
MOTA	638 OD1	ASN	79	15.291	52.886 120.43	5 1.00 12.93	${\tt HIGL}$
			79	15.353		1 1.00 12.14	HIGL
ATOM	639 ND2	ASN					HIGL
ATOM	640 C	ASN	79	13.111			· HIGL
MOTA	641 0	ASN	79	13.453	49.979 119.70	8 1.00 12.54	
ATOM	642 N	PHE	80	13.209	49.590 117.50	1.00 12.76	HIGL
	643 CA	PHE	80	13.752		1.00 13.01	HIGL
ATOM							HIGL
MOTA	644 CB	PHE	80	13.453			HIGL
MOTA	645 CG	PHE	80	12.076			
ATOM	646 CD1	PHE	80	11.636	45.998 117.12		HIGL
MOTA	647 CD2		80	11.218		4 1.00 12.89	HIGL
				10.363			HIGL
ATOM	648 CE1		80				HIGL
ATOM	649 CE2	PHE	80	9.943	3 46.692 115.04		

9.943 46.692 115.043 Fig. 2 cont.

				56	5/174		
ATOM	650 CZ	PHE .	80	9.517		1.00 13.02	HIGL
ATOM	651 C	PHE	80	15.259	48.253 117.690	1.00 13.33 1.00 14.29	HIGL HIGL
ATOM	652 O	PHE	80	15.937	48.944 116.940	1.00 14.29	HIGL
ATOM .	653 N	HIS	81.	15.784	47.499 118.649	1.00 12.98	HIGL
ATOM		HIS	. 81	17.227	47.426 118.823	1.00 13.89	HIGL
ATOM.	655 CB	HIS	81	17.626	47.425 120.304 48.782 120.933	1.00 15.21	HIGL
ATOM	656 CG	HIS	81	17.633	49.805 120.860	1.00 15.13	HIGL .
MOTA	657 CD2	HIS	81	16.749	49.204 121.777	1.00 15.56	HIGL
ATOM	658 ND1	HIS	81 81	18.639 18.375	50.429 122.196	1.00 14.49	HIGL
MOTA	659 CE1	HIS HIS	81	17.234	50.816 121.655	1.00 15.27	HIGL
ATOM	660 NE2 661 C	HIS	81	17.717	46.137 118.176	1.00 13.69	HIGL
ATOM ATOM	662 0	HIS	81	18.911	45.971 117.928	1.00 14.21	HIGL
MOTA	663 N	TYR	82 .	16.784	45.231 117.902	1.00 13.26	HIGL
ATOM	664 CA	TYR .	82	17.105	43.939 117.299	1.00 13.09	HIGL
ATOM	665 CB	TYR	.82	17.449	44.102 115.819	1.00 13.22	HIGL
ATOM	666 CG	TYR	82	16.277	44.556 114.986	1.00 13.70	HIGL
ATOM	667 CD1	TYR	82	15.014	43.977 115.161	1.00 13.38	HIGL HIGL
MOTA	668 CE1	TYR	82	13.939	44.348 114.378	1.00 12.96 1.00 12.39	HIGL
MOTA	669 CD2	TYR	82	16.429	45.529 114.002 45.908 113.209	1.00 12.39	HIGL
ATOM	670 CE2		82	15.359	45.310 113.400	1.00 13.13	HIGL
ATOM	671 CZ	TYR	82 82	14.114 13.046	45.652 112.595	1.00 15.86	HIGL
ATOM	672 OH 673 C	TYR TYR	62 62	18.257	43.278 118.030	1.00 13.08	$\mathtt{HIGL}$
ATOM ATOM	674 O	TYR	82	19.217	42.804 117.421	1.00 12.93	HIGL
ATOM	675 N	SER	83	18.137	43.256 119.352	1.00 13.03	HIGL
ATOM	676 CA	SER	83	19.132	42.668 120.227	1.00 13.56	HIGL
ATOM	677 CB	SER	83	20.266	43.671 120.439	1.00 13.70	HIGL
ATOM	678 OG	SER	83	21.309	43.114 121.210	1.00 15.51	HIGL
ATOM	679 C.	SER	83	18.440	42.348 121.557	1.00 14.03	HIGL HIGL
ATOM	680 O	SER	83 ·	17.332	42.827 121.805	1.00 13.59 1.00 14.12	HIGL
ATOM	681 N	ASP	84	19.066	41.532 122.405	1.00 14.12	HIGL
MOTA	682 CA	ASP	84	18.453	41.215 123.694 39.927 124.294	1.00 14.33	HIGL
ATOM	683 CB	ASP	84	19.025 18.577	38.682 123.558	1.00 16.47	HIGL
MOTA	684 CG	ASP	84 84	17.543	38.736 122.856	1.00 16.36	HIGL
MOTA	685 OD1	ASP ASP	84	19.259	37.643 123.704	1.00 17.16	HIGL
ATOM ATOM	687 C	ASP	84.	18.760	42.357 124.640	1.00 13.54	HIGL
MOTA	688 O	ASP	84	18.066	42.571 125.629	1.00 12.95	HIGL
ATOM	689 N	THR	85	19.806	43.100 124.308	1.00 12.90	HIGL
MOTA	690 CA .	THR	85	20.240	44.199 125.141	1.00 12.85	HIGL
ATOM	691 CB	THR	85	21.471	43.771 125.920	1.00 12.51	HIGL HIGL
MOTA	692 OG1	THR	85	21.661	44.642 127.038 43.810 125.013	1.00 14.10 1.00 12.87	HIGL
MOTA	693 CG2	THR	85	22.685	45.453 124.314	1.00 12.72	HIGL
MOTA	694 C	THR	85 85	20.555 20.377	45.463 123.095	1.00 12.75	HIGL
ATOM	695 O 696 N	THR TRP	86	21.038	46.495 124.989	1.00 11.76	HIGL
MOTA MOTA	697 CA	TRP	86	21.358	47.772 124.354	1.00 10.89	HIGL
ATOM	698 CB	TRP	86	22.198	48.651 125.276	1.00 9.89	HIGL
ATOM	699 CG	TRP	86	21.597	48.938 126.604	1,00 10.03	HIGL
ATOM	700 CD2	TRP	86	20.629	49.947 126.908	1.00 9.39	HIGL
ATOM	701 CE2	TRP	86	20.363	49.865 128.292	1.00 8.31	HIGL HIGL
MOTA	702 CE3	TRP	86	19.959	50.913 126.147	1.00 9.93	HIGL
MOTA	703 CD1	TRP	86	21.870	48.302 127.781	1.00 8.33 1.00 7.98	HIGL
ATOM	704 NE1	TRP	86	21.135	48.852 128.796 50.711 128.932		HIGL
ATOM	705 CZ2		86	19.457 19.051			HIGL
MOTA	706 CZ3		86 86	18.812			HIGL
ATOM	707 CH2 708 C	TRP	86	22.111			HIGL
ATOM ATOM	708 C	TRP	86	23.216		1.00 11.69	HIGL
ATOM	710 N	ALA	87	21.524	48.193 121.980	1.00 12.59	HIGL
ATOM	711 CA	ALA	87	22.189	48,180 120.685	1.00 12.82	HIGL
ATOM	712 CB	ALA	87	21.246	47.706 119.603	1.00 12.18	HIGL
ATOM	713 C	ALA	87	22.665		1.00 13.67	HIGL
ATOM	714 O	ALA	87	21.912	50.553 120.532	1.00 13.58	HIGL

Fig. 2 cont.

	,						
				_	/174		UTCI
MOTA	715 N	ASP	88	,	49.710 119.98	4 1.00 14.42 8 1.00 14.58	HIGL HIGL
ATOM	716 CA	ASP	88		50.984 119.62 51.744 120.88		HIGL
MOTA	717 CB	ASP	88	24.990 25.901	50.925 121.78		HIGL
MOTA	718 CG	ASP	88 88		50.268 121.26		HIGL
MOTA	719 OD1 720 OD2	ASP ASP	88	25.701	50.949 123.01	4 1.00 16.03.	HIGL
ATOM ATOM	720 OD2 721 C	ASP	88	25.721	50.691 118.69	0 1.00 15.64	HIGL
ATOM	722 0	ASP	88	26.023	49.529 118.41	1.00 15.14	HIGL
ATOM	723 N	PRO	89	26.408	51.734 118.19	92 1.00 16.24 05 1.00 16.14	HIGL HIGL
MOTA	724 CD	PRO	89	26.232	53.163 118.50 51.549 117.28		HIGL
MOTA	725 CA	PRO	89	27.545 28.119	52.954 117.15		HIGL
MOTA	726 CB 727 CG	PRO PRO	89 89	26.918	53.823 117.34		HIGL
ATOM .	727 CG 728 C	PRO	89 .	28.607	50.541 117.70	08 1.00 16.16	HIGL
MOTA	729 0	PRO	89	29.283	49.961 116.8		HIGL
ATOM	730 N	ALA	90	28.760	50.326 119.00		HIGL HIGL
MOTA	731 CA	ALA	90	29.773	49.387 119.46 50.003 120.5	62 1.00 16.48. 98 1.00 14.72	HIGL
MOTA	732 CB	ALA	90	30.596 29.191	48.054 119.8		HIGL
MOTA	733 C	ALA ·	90 90	29.939	47.143 120.2		HIGL
MOTA MOTA	734 O 735 N	HIS	91	27.867	47.933 119.8	89 1.00 15.05	HIGL
ATOM	736 CA	HIS	91	27.230	46.680 120.2	88 1.00 14.58	HIGL
MOTA	737 CB	HIS	91	26.897	46.673 121.7	85 1.00 15.34	HIGL HIGL
MOTA	738 CG	HIS	91	27.967	47,242 122.6 46,663 123.5	62 1.00 14.94 99 1.00 15.42	HIGL
ATOM	739 CD2	HIS	91	28.755 28.296	48.582 122.6		HIGL
MOTA	740 ND1 741 · CE1	HIS HIS	91 91	29.237	48,803 123.5	61 1.00 16.41	HIGL
ATOM ATOM	741 CE1	HIS	91	29.534	47,654 124.1	46 1.00 15.75	HIGL
ATOM	743 C	HIS	91	25.939	46.414 119.5	18 1.00 14.68	HIGL
ATOM	744 O	HIS	91	24.944	47,123 119.6	79 1.00 14.01 80 1.00 14.89	HIGL HIGL
ATOM	745 N	GLN	92	25.968	45.385 116.6 44.974 117.8		HIGL
MOTA	746 CA	GLN	92 92	24.818 25.000	45.394 116.4		HIGL
MOTA MOTA	747 CB 748 CG	GLN GLN	92	24.928	46.904 116.1	59 1.00 13.75	HIGL
ATOM	749 CD	GLN	92	23.529	47.497 116.3	368 1.00 13.63	HIGL
ATOM	750 OE1	GLN	92	22.517	46.899 115.9		HIGL HIGL
ATOM	751 NE2	GLN	92	23.475	48.685 116.9		HIGL
ATOM	752 C	GLN	92	24.786 24.994	43.451 118.0 42.721 117.0		HIGL
MOTA	753 O 754 N	GLN THR	92 93	24.530	42.984 119.2		HIGL
ATOM ATOM	755 CA	THR	93	24.510	41.561 119.5	520 1.00 14.27	HIGL
ATOM	756 CB	THR	93	24.672	41.329 121.0	1.00 14.39	HIGL
MOTA	757 OG1		93	25.783	42.100 121.4	497 1.00 13.20 315 1.00 12.37	HIGL HIGL
ATOM	758 CG2		93	24.906	39.842 121.3 40.838 119.0		HIGL
ATOM	759 C	THR	93 93	23.259 22.169	41.066 119.0		HIGL
MOTA MOTA	760 O 761 N	THR THR	94	23.428	39.951 118.	097 1.00 14.94	HIGL
ATOM	762 CA	THR	94	22.323	39.162 117.	576 1.00 15.30	HIGL
ATOM	763 CB	THR	94	22.818	38.169 116.	503 1.00 15.55	HIGL
ATOM	764 OG1		94	23.376	38.893 115.	399 1.00 15.22 013 1.00 15.52	HIGL HIGL
ATOM	765 CG2		94	21.677 21.720	37.302 116. 38.373 118.		HIGL
MOTA	766 C	THR	94 94	22.447	37.830 119.		HIGL
MOTA MOTA	767 O 768 N	THR PRO	95	20.381	38.309 118.	806 1.00 16.47	HIGL
ATOM	769 CD	PRO	95	19.409	38.946 117.	901 1.00 16.88	HIGL
MOTA	770 CA	PRO	95	19.695	37.573 119.	878 1.00 16.79	HIGL HIGL
MOTA	771 CB	PRO	95	18.220	37.690 119.	490 1.00 16.02 754 1.00 16.42	HIGL
ATOM	772 CG	PRO	95 05	18.161			HIGL
ATOM	773 C	PRO PRO	95 95	20.156 20.230			HIGL
ATOM ATOM	774 O 775 N	ALA	96	20.230	35.590 121.	073 1.00 17.31	HIGL
ATOM	776 CA	ALA	96	20.903	34.196 121.	149 1.00 17.43	HIGL
MOTA	777 CB	ALA	96	21.086	33.769 122.	598 1.00 17.13	HIGL HIGL
MOTA	778 C	ALA	96	19.821	33.356 120.	495 1.00 16.72 693 1.00 15.96	
MOTA	779 0	ALA	96	18.636	33.612 120.	7.00 TO.50	

Fig. 2 cont.

				58	3/174		
ATOM	780 N	GLY	97	20.229		1.00 17.32	HIGL
ATOM	781 CA	GLY	97	19.263		1.00 17.04	HIGL HIGL
ATOM	782 C	GLY	97	19.001	31.856 117.573 30.976 116.783	1.00 17.23 1.00 17.90	HIGL
MOTA	783 0	GLY	97	18.675 19.135	33.124 117.205	1.00 16.99	HIGL
ATOM	784 N	TRP TRP	98 98	18.907	33.524 115.820	1.00 17.97	HIGL
ATOM ATOM	785 CA 786 CB	TRP	98	18.901	35.051 115.726	1.00 18.18	$\mathtt{HIGL}$
ATOM	787 CG	TRP	98	17.627	35.621.116.258	1.00 18.37	HIGL
ATOM	788 CD2	TRP.	98 ·	17.022	36.870 115.907	1.00 18.66	HIGL HIGL
ATOM	789 CE2	TRP	98	15.824	36.978 116.650 37.909 115.036	1.00 18.98 1.00 18.95	HIGL
ATOM	790 CE3	TRP	98	17.372 16.798	35.041 117.175	1.00 18.96	HIGL
ATOM ATOM	791 CD1 792 NE1	TRP TRP	98 98	15.714	35.846 117.415	1.00 19.48	HIGL
ATOM	793 CZ2	TRP	98	14.973	38.083 116.550	1.00 18.24	HIGL
ATOM	794 CZ3	TRP .	98	16.521	39.011 114.936	1.00 18.88	HIGL
MOTA	795 CH2	TRP	98	15.336	39.085 115.690 32.897 114.877	1.00 18.43 1.00 17.57	HIGL
ATOM	796 C'	TRP	98	19.939 21.042	32.569 115.285	1.00 17.56	HIGL
MOTA	797 O 798 N	TRP · PRO	98 99	19.577	32.707 113.601	1.00 17.79	HIGL
ATOM ATOM	799 CD	PRO	99	18.219	32.889 113.063	1.00 17.38	HĮGL
ATOM	800 CA	PRO.	99	20.459	32.106 112.594	1.00 17.62	HÍGL
ATOM	801 CB	PRO	99	19.578	32.055 111.342	1.00 17.40 1.00 18.07	HIGL HIGL
ATOM	802 CG	PRO	99	18.491 21.842	33.041 111.616 32.693 112.326	1.00 18.07	HIGL
ATOM	803 C 804 O	PRO PRO	99 99	22.147	33.820 112.709	1.00 17.86	HIGL
ATOM ATOM	805 N	SER	100	22.670	31.887 111.660	1.00 17.52	$\mathtt{HIGL}$
MOTA	806 CA	SER	100	24.045	32.240 111.323	1.00 16.92	HIGL
ATOM	807 CB	SER	100	24.992	31.142 111.793	1.00 16.67 1.00 20.79	HIGL HIGL
ATOM	808 OG	SER	.100 100	24.564 24.283	30.601 113.025 32.452 109.833	1.00 16.73	HIGL
ATOM ATOM	809 C 810 O	SER SER	100	25.419	32.675 109.423	1.00 17.27	HIGL
ATOM	811 N	ASP	101	23.247	32.336 109.012	1.00 16.22	HIGL
ATOM	812 CA	ASP	101	23.422	32.564 107.579	1.00 16.38 1.00 16.22	HIGL HIGL
ATOM	813 CB	ASP	101	23.121 21.708	31.303 106.751 30.805 106.929	1.00 16.22	HIGL
MOTA	814 CG 815 OD1	ASP ASP	101 101	21.423	30.151 107.950	1.00 16.82	HIGL
MOTA MOTA	816 OD2	ASP	101	20.877	31.073 106.047	1.00 16.15	HIGL
MOTA	817 C	ASP	101	22.494	33.707 107.201	1.00 16.52	HIGL
ATOM	818 0	ASP	101	21.387	33.825 107.736 34.545 106.280	1.00 16.54 1.00 15.85	HIGL HIGL
ATOM	819 N	ILE	102 102	22.957 22.220	34.545 106.280 35.727 105.871	1.00 15.30	HIGL
ATOM ATOM	820 CA 821 CB	ILE.	102	22.958	36.484 104.746	1.00 14.62	HIGL
ATOM	822 CG2	ILE	102	22.862	35.709 103.433	1.00 14.59	HIGL
ATOM	823 CG1	ILE	102	22.361	37.884 104.594	1.00 13.26	HIGL
MOTA	824 CD1	ILE	102	22.438	38.731 105.856 35.519 105.452	1.00 10.57 1.00 16.31	HIGL HIGL
ATOM	825 C	ILE	102 102	20.779 19.929	36.365 105.739	1.00 17.53	HIGL
MOTA MOTA	826 O 827 N	ASN	102	20.486	34.409 104.784	1.00 15.84	HIGL
ATOM	828 CA	ASN	103	19.118	34.174 104.347	1.00 15.26	HIGL
ATOM	829 CB	ASN	103	19.056	33.026 103.345	1.00 16.44	HIGL HIGL
MOTA	830 CG	ASN	103	17.643	32.754 102.881 33.606 102.251	1.00 17.90 1.00 17.31	HIGL
ATOM	831 OD1		103 103	17.012 17.128	31.568 103.207	1.00 17.31	HIGL
ATOM ATOM	832 ND2 833 C	ASN ASN	103	18.195	33.872 105.520	1.00 14.76	HIGL
ATOM	834 0	ASN	103	17.081	34.390 105.592	1.00 14.43	HIGL
MOTA	835 ห	ASN	104	18.655		1.00 14.10	HIGL
MOTA	836 CA	ASN	104	17.849	32.684 107.598 31.424 108.277	1.00 13.79 1.00 13.76	HIGL
MOTA	837 CB 838 CG	ASN ASN	104 104	18.391 17.923		1.00 14.35	HIGL
ATOM ATOM	839 OD1		104	16.738	30.006 107.264	1.00 13.83	HIGL
ATOM	840 ND2		104	18.843	29.212 107.392	1.00 11.49	HIGL
MOTA	841 C	ASN	104	17.766	33.822 108.603	1.00 13.46 1.00 13.67	HIGL HIGL
ATOM	842 O	ASN	104	16.706 18.875			HIGL
MOTA MOTA	843 N 844 CA	LEU LEU	105 105	18.885			HIGL
FILOG	5.1.1 6.1				•		

Fig. 2 cont.

MOTA

909 CB

TYR

112

# 59/174 1.00 14.35 HIGL 36.256 109.855 20.282 105 LEU 845 CB ATOM 37.492 110.754 HIGL 1.00 15.28 20.373 105 ATOM 846 CG LEU 1.00 14.98 HIGL 37.133 112.168 19.941 847 CD1 105 LEU MOTA HIGL 1.00 15.43 38.025 110.756 105 21.791 848 CD2 LEU MOTA 36.694 109.291 1.00 15.25 HIGL 17.891 LEU 105 849 C MOTA HIGL 37.204 110.074 1.00 14.19 17.087 17.956 105 850 O LEU ATOM 37.009 108.000 1.00 15.85 HIGL 106 ALA ·851 N MOTA 1.00 17.40 HIGL 37.990 107.399 17.067 ATOM 852 CA ALA 106 38.177 105.916 37.532 107.548 1.00 15.61 HIGL 106 17.417 ATOM 853 CB ALA HIGL 1.00 18.34 15.618 106 854 C ALA ATOM HIGL 1.00 19.25 38.326 107.859 106 14.730 ALA 855 0 MOTA HIGL 1.00 19.52 36.245 107.320 15.390 ATOM 856 N 107 TRP HIGL 1.00 20.70 35.663 107.430 14.060 857 CA 107 TRP ATOM HIGL 34.177 107.104 1.00 22.69 14.140 107 TRP ATOM 858 CB 1.00 26.10 1.00 27.36 HIGL 33.566 106.709 12.847 107 859 'CG TRP ATOM HIGL 12.607 32.179 106.453 107 TRP MOTA 860 CD2 HIGL 32.056 106.055 1.00 28.11 107 11.256 ·861 CE2 ATOM TRP 1.00 27.84 HIGL 13.404 31.028 106.517 862 CE3 107 TRP MOTA 34.212 106.466 1.00 26.98 HIGL 11.665 863 CD1 107 TRP MOTA HIGL 1.00 27.36 33.310 106.072 10.705 107 864 NE1 TRP MOTA 1.00 28.94 1.00 28.94 HIGL 30.821 105.720 10.683 865 CZ2 107 ATOM TRP 29.804 106.184 HIGL 12.836 107 866 CZ3 TRP MOTA 29.711 105.790 HIGL 1.00 28.79 11.487 107 TRP MOTA 867 CH2 1.00 20.80 1.00 19.49 1.00 20.81 HIGL 13.567 35.862 108.862 868 C TRP 107 MOTA HIGL 36.280 109.097 35.567 109.812 12.428 107 TRP MOTA 869 O HIGL 14.453 108 870 N LYS ATOM 1.00 20.77 HIGL 35.707 111.231 14.158 108 MOTA 871 CA LYS 1.00 21.15 HIGL 35.255 112.070 15.358 872 CB 108 LYS ATOM 1.00 22.88 1.00 23.37 HIGL 34.250 113.161 15.018 108 MOTA 873 CG LYS HIGL 34.770 114.100 13.942 108 874 CD LYS MOTA 1.00 23.83 HIGL 33.698 115.088 13.525 108 MOTA 875 CE . LYS 1.00 24.90 HIGL 34.107 115.853 12.322 108 876 NZ LYS ATOM 1.00 19.90 HIGL 37.161 111.554 13.830 108 MOTA 877 C LYS 1.00 20.08 HIGL 37.450 112.214 12.836 108 878 O LYS ATOM 1.00 19.75 HIGL 38.074 111.094 14.674 109 MOTA 879 N LEU 1.00 19.93 HIGL 39.488 111.344 14.445 880 CA LEU 109 ATOM 1.00 17.82 1.00 17.82 HIGL 40.337 110.654 109 15.508 881 CB LEU MOTA HIGL 41.827 110.968 15.390 LEU 109 B82 CG MOTA 1.00 16.38 HIGL 42.054 112.449 15.672 16.368 109 883 CD1 LEU ATOM 1.00 16.81 HIGL 42.620 110.103 884 CD2 LEU 109 MOTA HIGL 1.00 20.34 1.00 20.28 39.861 110.822 109 13.063 885 C LEU MOTA 40.679 111.423 39.247 109.704 HIGL 12.362 886 0 109 LEU ATOM 1.00 20.51 HIGL 12.679 11.377 110 887 N TYR MOTA HIGL 39.489 109.100 38.862 107.704 1.00 20.92 110 888 CA TYR MOTA HIGL 1.00 21.24 11.309 110 889 CB TYR ATOM HIGL 38.842 107.101 37.757 107.292 1.00 21.40 9.918 890 CG 110 TYR MOTA 1.00 22.61 HIGL 9.064 110 891 CD1 TYR MOTA 37.748 106.754 39.922 106.358 39.926 105.817 HIGL 1.00 22.76 7.771 TYR 110 892 CE1 MOTA 1.00 23.16 HIGL 9.445 893 CD2 TYR 110 MOTA 1.00 22.90 HIGL 8.155 894 CE2 110 MOTA TYR 38.838 106.018 1.00 23.09 HIGL 7.325 110 895 CZ TYR ATOM HIGL 1.00 22.70 38.849 105.482 6.056 110 TYR ATOM 896 OH 1.00 21.45 HIGL 38.938 109.972 10.249 897 C TYR 110 ATOM HIGL 39.671 110.303 1.00 22.10 110 9.312 898 O ATOM TYR 1.00 20.73 HIGL 37.659 110.344 37.073 111.182 10.326 899 N ASN 111 ATOM HIGL 1.00 20.87 9.281 111 900 CA ASN MOTA HIGL 1.00 23.22 35.619 111.546 9.589 ASN 111 901 CB ATOM HIGL 34.699 110.348 1.00 26.49 9.612 902 CG 111 ASN ATOM 1.00 27.21 HIGL 35.005 109.301 9.040 903 ODI ASN 111 ATOM HIGL 33.552 110.516 1.00 29.16 10.265 904 ND2 111 ASN ATOM 1.00 19.60 HIGL 37.864 112.474 9.147 905 C ASN 111 ATOM HIGL 1.00 19.02 38.190 112.905 8.039 111 906 O ASN ATOM 1.00 18.21 HIGL 38.169 113.084 10.288 TYR 112 907 N MOTA HIGL 1.00 16.83 38.905 114.337 10.310 112 908 CA TYR ATOM HIGL 39.129 114.810 1.00 16.36

Fig. 2 cont.

11.751

# 60/174 40.071 115.991 1.00 14.95 HIGL 11.839 112 MOTA 910 CG TYR 1.00 15.11 HIGL 39.691 117.245 11.369 112 911 CD1 TYR MOTA 1.00 14.94 HIGL 40.581 118.316 112 11.369 MOTA 912 CE1 TYR HIGL 41.366 115.836 1.00 14.45 12.319 913 CD2 TYR 112 MOTA 42.264 116.897 1.00 14.83 HIGL 12.323. TYR 112 914 CE2 MOTA HIGL 11.847 .41,866 118,133 1.00 14.96 112 915 CZ TYR ATOM 1.00 15.27 1.00 16.36 HIGL 42.754 119.182 11.848 112 MOTA 916 OH TYR HIGL 40.243 114.224 9.601 112 917 C TYR. ATOM 1.00 15.41 40.534 114.999 HIGL 8.686 112 918 O TYR ATOM 1.00 16.21 HIGL 41.056 113.265 10.034 113 919 N THR ATOM 1.00 15.87 1.00 16.16 42.369 113.058 HIGL 9.443 113 ATOM 920 CA THR 43.125 111.922 HIGL 10.142 113 921 CB THR MOTA HIGL 43.252 112.221 1.00 15.12 11.537 THR 113 922 OG1 MOTA 1.00 15.98 44.515 111.758 .42.216 112.717 HIGL 9.537 923 CG2 THR 113 ATOM 1.00 16.24 1.00 16.57 HIGL 973. ٢ 113 924 C THR MOTA HIGL 42.896 113.290 7.124 ATOM. 925 O THR 113 1.00 16.92 HIGL 41.307 111.790 7.678 114 ATOM LEU 926 N HIGL 1.00 16.65 6.304 41.043 111.366 MOTA 927 CA LEU 114 1.00 15.97 1.00 16.54 39.849 110.411 HIGL 928 CB 114 6.264 LEU ATOM HIGL 4.861 39.423 109.964 ATOM 929 CG LEU 114 1.00 15.93 1.00 14.91 HIGL 40.543 109.154 930 CD1 LEU 114 4.220 MOTA HIGL 38.144 109.146 4.948 114 ATOM 931 CD2 LEU 40.754 112.565 1.00 16.56 HIGL 5.404 932 C LEU 114 ATOM 1.00 16.01 HIGL 4.420 41.450 112.799 114 MOTA 933 0 LEU 39.720 113.320 1.00 16.95. HIGL 5.749 ATOM 934 N ASP 115 1.00 17.44 HIGL 4.967 39.347 114.484 115 ASP ATOM 935 CA HIGL 1.00 18.68 5.562 38.104 115.139 936 CB 115 MOTA ASP 1.00 20.91 HIGL 5.489 36.884 114.235 ASP 115 ATOM 937 CG HIGL 1.00 20.18 37.019 113.095 4.994 ATOM 115 938 OD1 ASP 1.00 22.87 1.00 17.05 HIGL 35.789 114.658 5.928 115 ASP ATOM 939 OD2 40.481 115.491 40.732 116.048 HIGL 4.879 940 C ASP 115 ATOM 1.00 16.42 HIGL 3.813 941 0 ASP 115 MOTA 1.00 16.71 1.00 17.19 1.00 17.37 41.174 115.713 HIGL 5.990 942 N SER 116 ATOM 42.279 116.660 HIGL 116 6.005 ATOM 943 CA SER 42.869 116.774 41.969 117.391 HIGL 7.409 116 MOTA 944 CB SER 1.00 17.53 HIGL 8.307 945 OG SER 116 MOTA 1.00 18.12 HIGL 5.023 43.381 116.262 946 C SER 116 ATOM 43.847 117.084 43.812 115.008 1.00 17.59 HIGL 4.231 116 947 0 SER MOTA 1.00 18.86 HIGL 5.080 117 MET MOTA 948 N 44.856 114.552 HIGL 1.00 19.77 4.176 949 CA MET 117 ATOM 1.00 19.25 1.00 18.96 1.00 20.56 45.262 113.125 45.989 113.006 47.687 113.654 HIGL 4.525 117 950 CB MET MOTA HIGL 5.862 MET 117 ATOM 951 CG HIGL 5.846 117 ATOM 952 SD MET 1.00 20.80 1.00 20.69 HIGL 6.173 47.395 115.398 953 CE MET 117 MOTA HIGL 2.729 44.384 114.641 117 954 C MET ATOM HIGL 1.00 19.86 45.134 115.056 1.843 MOTA 955 O MET 117 1.00 22.17 HIGL 43.132 114.266 2.488 ASN 118 956 N MOTA HIGL 1.00 23.55 42.589 114.327 957 CA 958 CB 1.137 ASN 118 MOTA 1.00 22.99 1.00 24.24 HIGL 41.192 113.704 118 1.081 ASN MOTA 41.236 112.197 HIGL 0.966 959 CG ASN 118 MOTA 1.00 24.38 1.00 25.71 HIGL 42.054 111.648 960 OD1 118 0.231 ASN MOTA HIGL 40.345 111.516 1.680 ATOM 961 ND2 ASN 118 1.00 24.12 HIGL 42.536 115.772 0.665 962 C 118 ASN MOTA 42.535 116.054 42.501 116.691 1.00 24.65 HIGL -0.532 118 MOTA 963 0 ASN 1.00 25.04 HIGL 119 1.617 964 N ARG ATOM 1.00 25.97 HIGL 1.289 42.457 118.104 119 965 CA MOTA ARG 1.00 27.25 1.00 30.86 HIGL 42.289 118.916 2.564 966 CB ARG 119 ATOM HIGL 2.324 41.905 120.343 ARG 119 MOTA 967 CG 1.00 32.19 40.518 120.464 HIGL 968 CD ARG 119 MOTA 1.00 35.20 HIGL 1.381 40,252 121.856 119 MOTA 969 NE ARG 1.00 35.79 HIGL 40.036 122.826 MOTA 970 CZ ARG 119 2.266 HIGL 1.00 35.68 3.566 40.038 122.564 119 ARG ATOM 971 NH1 HIGL 39.846 124.070 1.00 37.32 119 1.845 972 NH2 ARG ATOM HIGL 1.00 26.06 43.755 118.483 0.572 119 MOTA 973 C ARG

Fig. 2 cont.

43.744 119.234

1.00 26.17

HIGL

-0.406

974 0

ATOM

ARG

119

				6	1/174		
ATOM	975 ห	PHE	120	1.058	44.874 117.952	1.00 25.97	HIGL
ATOM	976 CA	PHE	120	0.438	46.166 118.218	1.00 25.91	HIGL
ATOM	977 CB	PHE	120 120	1.369 2.516	47.312 117.811 47.519 118.748	1.00 24.71 1.00 23.82	HIGL HIGL
ATOM ATOM	978 CG 979 CD1	PHE ·	120	3.748	46.923 118.508	1.00 24.05	HIGL
ATOM	980 CD2	PHE	120	2.356	48.289 119.892	1.00 23.49	HIGL
'ATOM	981 CE1	PHE	120	4.806	47.088 119.396	1.00 23:14	HIGL
ATOM	982 CE2	PHE	120	3.407	48.461 120.788 47.860 120.540	1.00 23.31 1.00 23.49	HIGL HIGL
MOTA MOTA	983 CZ 984 C	PHE PHE	120 120	4.632 -0.879	46.283 117.452	1.00 26.35	HIGL
ATOM	985 O	PHE	120	-1.879	46.758 117.988	1.00 26.78	HIGL
MOTA	986 N	ALA	121	-0.870	45.844 116.198	1.00 26.40	HIGL
ATOM	987 CA	ALA	121	-2.058 -1.755	45.891 115.357 45.280 114.003	1.00 26.80 1.00 27.18	HIGL HIGL
ATOM ATOM	988 CB 989 C	ALA ALA	121 121	-3.211	45.143 116.016	1.00 27.34	HIGL
MOTA	990 0	ALA	121	-4.314	45.674 116.152	1.00 27.77	HIGL
ATOM	991 N	ASP	122	-2.948	43.905 116.423	1.00 26.89	HIGL HIGL
MOTA	992 CA 993 CB	ASP ASP	122 122	-3.965 -3.436	43.084 117.063 41.665 117.303	1.00 26.21 1.00 25.67	HIGL.
ATOM ATOM	994 CG	ASP	122	-3.074	40.950 116.012	1.00 25.38	HIGL
ATOM	995 OD1	ASP	122	-3.544	41.379 114.929	1.00 24.57	HIGL
ATOM	996 OD2	ASP	122	-2.328	39.950 116.069	1.00 24.15 1.00 26.13	HIGL HIGL
MOTA MOTA	997 C. 998 O	ASP ASP	122 122	-4.414 -5.549	43.686 118.389 43.478 118.822	1.00 26.13	HIGL
MOTA	999 N	ALA .	123	-3.517	44.427 119.033	1.00 24.90	HIGL
ATOM	1000 CA	ALA	123	-3.821	45.053 120.308	1.00 22.75	HIGL
ATOM	1001 CB 1002 C	ALA ALA	123 123	-2.548 -4.595	45.330 121.058 46.344 120.102	1.00 23.23 1.00 22.12	HIGL HIGL
ATOM ATOM	1002 C	ALA	123	-5.085	46.935 121.058	1.00 22.33	HIGL
ATOM	1004 N	GLY	124	-4.704	46.778 118.850	1.00 21.85	
MOTA	1005 CA	GLY	124	-5.424 -4.604	48.002 118.548 49.253 118.809	1.00 21.93 1.00 22.90	HIGL HIGL
ATOM ATOM	1006 C 1007 O	GLY GLY	124 124	-5.150	50.350 118.957	1.00 22.21	HIGL
MOTA	1008 N	ILE	125	-3.286	49.078 118.876	1.00 23.51	HIGL
MOTA	1009 CA	ILE	125	-2.352	50.174 119.113 49.706 119.949	1.00 23.71 1.00 24.28	HIGL HIGL
ATOM ATOM	1010 CB 1011 CG2	ILE	125 125	-1.132 -0.171	50.871 120.153	1.00 24.28	HIGL
ATOM	1012 CG1	ILE	125	-1.587	49.094 121.283	1.00 24.08	HIGL
ATOM	1013 CD1	ILE	125	-2.168	50.078 122.258	1.00 24.75 1.00 24.07	HIGL HIGL
ATOM ATOM	1014 C 1015 O	ILE	125 125	-1.817 -1.416	50.648 117.765 49.837 116.939	1.00 24.23	HIGL
ATOM	1016 N	GLN	126	-1.805	51.952 117.533	1.00 24.42	HIGL
MOTA	1017 CA	GLN .	126	-1.282	52.451 116.274	1.00 25.40	HIGL
ATOM ATOM	1018 CB 1019 CG	GLN GLN	126 126	-2.112 -1.591	53.631 115.766 54.243 114.464	1.00 26.92 1.00 29.76	HIGL HIGL
ATOM	1019 CG 1020 CD	GLN	126	-1.473	53.223 113.329	1.00 32.33	HIGL
ATOM	1021 OE1	GLN	126	-2.456	52.570 112.953	1.00 33.86	HIGL
MOTA	1022 NE2	GLN	126	-0.267	53.086 112.777	1.00 31.82 1.00 25.09	HIGL HIGL
ATOM A'FOM	1023 C 1024 O	GLN GLN	126 126	0.174 0.494	52.883 116.424 53.731 117.260	1.00 25.29	HIGL
ATOM	1025 N	VAL	127	1.046	52.280 115.617	1.00 23.64	HIGL
MOTA	1026 CA	JAV	127	2.465	52.605 115.614	1.00 21.87	HIGL
ATOM ATOM	1027 CB 1028 CG1	VAL VAL	127 127	3.329 4.800	51.373 115.255 51.730 115.338	1.00 21.30 1.00 20.09	HIGL HIGL
ATOM	1028 CG1	VAL	127	3.010	50.217 116.184	1.00 20.69	HIGL
ATOM	1030 C	VAL	127	2.635	53.658 114.526	1.00 21.93	HIGL
ATOM	1031 O	VAL	127 128	2.268	53.427 113.378 54.809 114.882	1.00 22.89 1.00 21.66	HIGL HIGL
MOTA MOTA	1032 N 1033 CA	ASP ASP	128	3.192 3.378	55.896 113.927	1.00 21.00	HIGL
ATOM	1034 CB	ASP	128	3.080	57.211 114.628	1.00 21.65	HIGL
MOTA	1035 CG	ASP	128	1.662	57.260 115.145	1.00 22.08	HIGL HIGL
ATOM ATOM	1036 OD1 1037 OD2	ASP ASP	128 128	0.744 1.458	57.299 114.301 57.231 116.380	1.00 23.35 1.00 22.69	HIGL
ATOM	1038 C	ASP	128	4.746	55.932 113.256	1.00 21.00	HIGL
ATOM	1039 0	ASP	128	4.854	56.276 112.077	1.00 20.64	HIGL
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Fig. 2 cont.

				6	2/174		
MOTA	1040 N	ILE	129	5.786	55.587 114.010	1.00 19.93	HIGL
ATOM	1041 CA	ILE	129	7.139	55.535 113.472	1.00 18.94	HIGL
MOTA	1042 CB.	ILE	129	7.999	56.721 113.927	1.00 17.89	HIGL HIGL
ATOM	1043 CG2		129	9.425	56.533 113.444	1.00 16.07 1.00 17.25	HIGL
MOTA	1044 CG1	ILE	129	7.440	58.027 113.375	1.00 17.25	HIGL
ATOM	1045 CD1	ILE	129	8.207	59.241 113.843 54.267 113.985	1.00 19.57	HIGL
MOTA	1046 C	ILE	129 129	7.808 7.591	53.867 115.130	1.00 20.12	HIGL
ATOM	1047 O 1048 N	ILE VAL	130	8.614	53.640 113.133	1.00 19.09	HIGL
ATOM ATOM	1046 N 1049 CA	VAL	130	9.343	52.430 113.497	1.00 18.61	HIGL
ATOM	1050 CB	VAL	130	8.734	51.154 112.868	1.00 19.46	HIGL
ATOM	1051 CG1	VAL	130	9.424	49.923 113.431	1.00 18.88	HIGL
ATOM	1052 CG2	VAL	130	7.255	51.087 113.133	1.00 21.50	HIGL
ATOM	1053 C	VAL	130	10.762	52.531 112.962	1.00 17.57	HIGL HIGL
MOTA	1054 O	VAL	130	10.962	52.707 111.759	1.00 17.98	HIGL
ATOM	1055 N	SER	131	11.749	52.439 113.843	1.00 15.84 1.00 14.70	HIGL
MOTA	1056 CA	SER	131	13.127 14.038	52.470 113.377 53.282 114.314	1.00 14.70	HIGL
MOTA	1057 CB 1058 OG	SER SER	131	14.319	52.589 115.514	1.00 18.11	HIGL
ATOM ATOM	1058 OG 1059 C	SER	131	13.565	51.018 113.345	1.00 12.96	HIGL
ATOM	1060 0	SER	131	13.436	50.299 114.335	1.00 11.68	HIGL
MOTA	1061 N	ILE	132	14.039	50.572 112.191	1.00 10.75	HIGL
ATOM	1062 CA	ILE	132	14.492	49.207 112.073	1.00 10.19	HIGL
ATOM	1063 CB	ILE	132	14.319	48.707 110.632	1.00 10.00	HIGL
MOTA	1064 CG2	ILE	132	12.858	48.371 110.380	1.00 9.71 1.00 10.09	HIGL HIGL
ATOM	1065 CG1	ILE	132	14.785	49.781 109.646 49.350 108.198	1.00 10.09	HIGL
MOTA	1066 CD1	ILE	132 132	14.716 15.954	49.155 112.508	1.00 10.16	HIGL
ATOM ATOM	1067 C 1068 O	ILE	132	16.869	49.045 111.693	1.00 9.89	HIGL
ATOM	1069 N	GLY	133	16.160	49.253 113.814	1.00 9.99	HIGL
ATOM	1070 CA	GLY	133	17.500	49.230 114.364	1.00 10.91	HIGL
MOTA	1071 C	.GLY	. 133	17.711	50.461 115.220	1.00 11.73	HIGL
ATOM	1072 O	GLY	133	16.885	51.378 115.193	1.00 11.22	HIGL
ATOM	1073 N	ASN	134	18.804	50.482 115.983	1.00 11.81	HIGL HIGL
ATOM	1074 CA	ASN	134	19.119	51.621 116.843 51.271 118.307	1.00 11.67 1.00 11.03	HIGL
ATOM	1075 CB 1076 CG	ASN ASN	134 134	18.878 19.010	52.481 119.217	1.00 11.61	HIGL
MOTA MOTA	1076 CG 1077 OD1	ASN	134	18.116	53.328 119.269	1,00 9.26	HIGL
ATOM	1078 ND2	ASN	134	20.140	52.579 119.923	1.00 10.03	HIGL
ATOM	1079 C	ASN	134	20.578	52.041 116.673	1.00 12.23	HIGL
ATOM	1080 O	ASN	134	21.488	51.299 117.047	1.00 12.50	HIGL
MOTA	1081 N	GLU	135	20.796	53.237 116.130	1.00 12.34	HIGL
ATOM	1082 CA	GLU	135	22.148	53.745 115.905	1.00 12.34 1.00 12.86	HIGL HIGL
ATOM	1083 CB	GLU	135	22.819	54.137 117.233 55.229 118.021	1.00 12.86	HIGL
ATOM ATOM	1084 CG 1085 CD	GLU GLU	135 135	22.107 22.988	55.855 119.109	1.00 14.70	HIGL
MOTA	1085 CD	GLU	135	23.605	55.107 119.895	1.00 13.98	HIGL
ATOM	1087 OE2	GLU	135	23.059	57.100 119.186	1.00 14.17	HIGL
ATOM	1088 C	GLU	135	22.980	52.662 115.217	1.00 11.83	HIGL
MOTA	1089 O	GLU	135	24.062	52.307 115.689	1.00 11.40	HIGL
ATOM	1090 N	ILE	136	22.464	52.139 114.107	1.00 11.55	HIGL
MOTA	1091 CA	ILE	136	23.145	51.086 113.366	1.00 12.33 1.00 11.21	HIGL HIGL
MOTA	1092 CB	ILE	136	22.134	50.255 112.537 49.523 113.478	1.00 11.21	HIGL
ATOM	1093 CG2 1094 CG1	ILE	136 136	21.187 21.346	51.166 111.583	1.00 10.88	HIGL
MOTA MOTA	1094 CG1	ILE	136	20.307	50.439 110.712	1.00 5.41	HIGL
MOTA	1095 CDI	ILE	136	24.272	51.570 112.446	1.00 13.31	HIGL
ATOM	1097 0	ILE	136	24.512	50.981 111.397	1.00 13.57	HIGL
ATOM	1098 N	THR	137	24.978	52.621 112.860	1.00 14.02	HIGL
ATOM	1099 CA	THR	137	26,076	53.177 112.073	1.00 15.42	HIGL
ATOM	1100 CB	THR	137	26.796		1.00 15.31	HIGL HIGL
MOTA	1101 OG1	THR	137	25.835	55.190 113.390	1.00 15.48 1.00 13.55	HIGL
ATOM	1102 CG2	THR	137 137	27.705 27.128		1.00 13.33	HIGL
ATOM ATOM	1103 C 1104 O	THR THR	137	27.126		1.00 17.91	HIGL
U T OLI	1104 0	LIII		2.,070		··	

Fig. 2 cont.

# 63/174 1.00 17.23 HIGL 51.214 112.596 27.421 138 GLN 1105 N ATOM 50.166 112.308 1.00 17.23 HIGL 28,396 138 1106 CA GLN MOTA HIGL 49.926 113.503 1.00 18.55 29.328 138 1107 CB GLN ATOM 1.00 22.06 51.101 113.856 HIGL 138 30.240 1108 CG GLN **ATOM** 1.00 24.27 HIGL 51.687 112.642 30.963 1109 CD 138 GLN ATOM 1.00 24.26 HIGL 50.975 111.897 31.641 138 MOTA 1110 OE1 GLN 1.00 24.87 HIGL 30.821 52.997 112.445 138 1111 NE2 GLN ATOM 1.00 16.30 1.00 15.80 48.886 111.985 HIGL 27.633 138 ATOM 1112 C GLN HIGL 28.133 47.774 112.187 138 1113 0 GLN ATOM 1.00 14.43 HIGL 49.059 111.490 139 26.411 MOTA 1114 N GLY 1.00 14.15 HIGL 47.917 111.138 25.590 1115 CA GLY 139 MOTA 1.00 13.48 1.00 11.76 HIGL 24.778 47.376 112.304 139 MOTA 1116 C GLY 48.001 113.363 HIGL 24.703 1117 0 GLY 139 ATOM 1.00 12.77 HIGL 24.175 23.353 46.207 112.098 14Ó 1118 N LEU ATOM 1.00 12.79 : HIGL 45.562 113.114 1119 CA LEU 140 ATOM 1.00 12.46 HIGL 45.922 112.917 140 21.878 1120 CB LEU MOTA 45.335 111.695 1.00 i2.85 HIGL. 21.162 1121 CG LEU 140 MOTA 1.00 13.35 HIGL 140 19.672 45.582 111.817 MOTA 1122 CD1 LEU HIGL 45.954 110.416 1.00 12.87 21.687 140 1123 CD2 LEU ATOM 1.00 13.36 HIGL 44.055 113.010 140 23.504 1124 C LEU MOTA HIGL 43.554 112.072 1.00 13.25 24.120 140 **ATOM** 1125 0 LEU 1.00 13.28 HIGL 43.342 113.980 22.937 141 1126 N LEU MOTA HIGL 1.00 12.60 22.975 41.883 114.008 141 1127 CA LEU ATOM 1.00 10.91 HIGL 41.340 113.069 21.895 141 ATOM 1128 CB LEU 41.627 113.587 HIGL 20.481 1.00 10.89 141 LEU 1129 CG ATOM 9.50 HIGL 1.00 19.432 41.270 112.543 141 1130 CD1 LEU MOTA HIGL 8.29 1.00 40.846 114.880 20.264 1131 CD2 141 LEU MOTA 1.00 13.21 HIGL 24.337 41.284 113.656 141 1132 C LEU ATOM HIGL 1.00 14.64 24.462 40.504 112.708 141 LEU 1133 0 MOTA 1.00 13.26 HIGL 25.353 26.705 41.644 114.432 142 ATOM 1134 N TRP HIGL 41.149 114.204 · 1.00 13.14 142 1135 CA TRP MOTA 1.00 11.33 HIGL 27.686 41.859 115.130 142 1136 CB TRP MOTA HIGL 43.330 114.910 44.272 115.695 1.00 10.90 27.757 1137 CG 142 TRP MOTA 1.00 11.10 HIGL 28.488 142 MOTA 1138 CD2 TRP HIGL 1.00 11.19 45.545 115.113 142 28.289 1139 CE2 TRP MOTA 1.00 10.40 1.00 10.69 1.00 10.00 HIGL 142 29.290 44.167 116.835 TRP MOTA 1140 CE3 44.046 113.911 HIGL 27.158 1141 CD1 142 TRP MOTA HIGL 27.474 45.379 114.025 142 MOTA 1142 NE1 TRP1.00 11.44 HIGL 46.705 115.635 28.869 1143 CZ2 TRP 142 MOTA 1.00 11.67 45.319 117.353 46.573 116.750 HIGL 29.863 142 MOTA 1144 CZ3 TRP 29.650 26.768 26.046 HIGL 1.00 11.55 1145 CH2 TRP 142 MOTA 1.00 13.84 HIGL 142 39.652 114.442 TRP MOTA 1146 C 39.126 115.286 1.00 14.95 HIGL 1147 O TRP 142 MOTA 1.00 13.87 1.00 13.74 HIGL 38.952 113.751 143 27.680 PRO ATOM 1148 N 37.534 114.052 39.417 112.776 HIGL 27.900 PRO 143 MOTA 1149 CD 1.00 14.76 HIGL 143 28.675 PRO 1150 CA MOTA HIGL 29.669 38.253 112.701 1.00 13.49 PRO 143 MOTA 1151 CB 1.00 13.80 HIGL 37.438 113.918 143 29.386 1152 CG PRO ATOM HIGL 1.00 15.67 28.174 39.778 111.381 1153 C PRO 143 MOTA HIGL 28.703 27.182 1.00 16.90 40.693 110.755 143 PRO ATOM 1154 O HIGL 39.044 110.887 1.00 15.74 1155 N 144 LEU MOTA 1.00 16.05 HIGL 39.272 109.549 26.648 144 ATOM 1156 CA LEU HIGL 38.459 109.358 1.00 15.16 25.366 1157 CB 144 LEU MOTA 1.00 14.79 HIGL 25.558 24.214 36.942 109.467 LEU 144 1158 CG MOTA HIGL 1.00 14.16 36.248 109.414 1159 CD1 1160 CD2 144 LEU MOTA 1.00 14.04 1.00 17.32 HIGL 26.455 36.449 108.331 144 FEU MOTA HIGL 26.397 26.911 40.727 109.159 144 1161 C LEU ATOM 41.191 108.144 1.00 17.71 144 MOTA 1162 O **LEU** 41.451 109.956 HIGL 1.00 17.84 25.617 GLY 145 1163 N MOTA 1.00 17.98 HIGL 145 25.325 42.835 109.617 1164 CA GLYMOTA 1.00 18.71 HIGL 43.888 110.051 26.335 GLY 145 1165 C ATOM 1.00 19.15 HIGL 26.008 45.077 110.123 1166 O GLY 145 ATOM 1.00 18.29 HIGL 43.477 110.341 27.560 LYS 146 1167 N MOTA 1.00 19.30 HIGL 44.428 110.762 28.575 146 MOTA 1168 CA LYS 1.00 18.95 HIGL 43.687 111.423 29.733

Fig. 2 cont.

LYS

1169 CB

ATOM

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					1/174		
ATOM	1170 CG	LYS	146	30.533		1.00 18.69	HIGL
ATOM	1171 CD	LYS	146	31.624		1.00 20.37 1.00 20.86	HIGL HIGL
MOTA	1172 CE	LYS	146	32.528		1.00 20.66	HIGL
MOTA	1173 NZ	LYS	146	31.799 29.062		1.00 20.47	HIGL
ATOM	1174 C	LYS LYS	146 146	29.062	44.685 108.453	1.00 19.27	HIGL
MOTA MOTA	1175 O 1176 N	THR	147	29.312	46.519 109.752	1.00 21.74	HIGL
MOTA	1177 CA	THR	147	29.746	47.374 108-659	1.00 23.27	HIGL
ATOM	1178 CB	THR	147	30.212		1.00 22.61	HIGL HIGL
MOTA	1179 OG1	THR	147	30.794	48.619 110.430 49.703 109.127	1.00 23.56 1.00 23.05	HIGL
MOTA	1180 CG2	THR	147	29.050 30.817	46.833 107.747	1.00 24.76	HIGL
ATOM ATOM	1181 C 1182 O	THR THR	147 147	31.763	46.161 108.173	1.00 24.27	HIGL
ATOM	1182 U	ASN	148	30.631	47.193 106.478	1.00 26.25	HIGL
MOTA	1184 CA	ASN	148	31.456	46.818 105.346	1.00 26.20	HIGL HIGL
MOTA	1185 CB	ASN	148	32.917	46.692 105.763	1.00 26.56 1.00 26.62	HIGL
MOTA	1186 CG	ASN	148	33.560 32.903	48.057 105.998 48.985 106.472	1.00 26.32	HIGL
MOTA	1187 OD1 1188 ND2	asn asn	148 148	34.842	48.183 105.670	1.00 25.69	HIGL
ATOM ATOM	1189 C	ASN	148	30.865	45.542 104.762	1.00 26.28	HIGL
ATOM	1190 0	ASN	148	31.279	45.076 103.707	1.00 28.00	HIGL
ATOM	1191 N	ASN	149	29.873	44.998 105.464	1.00 25.38 1.00 24.20	HIGL HIGL
MOTA	1192 CA	ASN	149	29.127 28.733	43.826 105.007 42.927 106.177	1.00 24.20	HIGL ·
MOTA	1193 CB	asn Asn	149 149	29.858	42,016 106.615	1.00 24.57	HIGL
MOTA MOTA	1194 CG 1195 OD1	ASN	149	31.033	42,309 106.391	1.00 25.70	HIGL
ATOM	1196 ND2	ASN	149	29.505	40.910 107.260	1.00 23.86	HIGL
MOTA	1197 C	ASN	149	27.877	44.466 104.421	1.00 23.50 1.00 24.05	HIGL HIGL
MOTA	1198 0	ASN	149	26.753	44.012 104.637 45.554 103.698	1.00 21.67	HIGL
ATOM	1199 N 1200 CA	TRP TRP	150 150	28.101 27.039	46.323 103.079	1.00 20.87	HIGL
ATOM ATOM	1200 CA 1201 CB	TRP	150	27.649	47,265 102.045	1.00 19.65	HIGL
ATOM	1202 CG	TRP	150	28.654	48.200 102.653	1.00 19.10	HIGL HIGL
ATOM	1203 CD2	TRP	150	28.411	49.153 103.697	1.00 19.28 1.00 18.98	HIGL
ATOM	1204 CE2	TRP	150	29.631 27.278	49.828 103.938 49.506 104.452	1.00 18.67	HIGL
ATOM ATOM	1205 CE3 1206 CD1	TRP TRP	150 150	29.976	48.329 102.315	1.00 18.26	HIGL
ATOM	1200 CD1	TRP	150	30.567	49.306 103.080	1.00 17.94	HIGL
ATOM	1208 CZ2	TRP	150	29.751	50.837 104.902	1.00 19.36	${\tt HIGL}$
MOTA	1209 CZ3	TRP	150	27.395	50.506 105.409 51.162 105.626	1.00 19.12 1.00 19.64	HIGL
ATOM	1210 CH2	TRP TRP	150 150	28.627 25.939	45.479 102.451	1.00 20.95	HIGL
MOTA MOTA	1211 C 1212 O	TRP	150	24.757	45.801 102.583	1.00 21.08	HIGL
MOTA	1213 N	TYR	151	26.315	44.400 101.769	1.00 20.56	HIGL
ATOM	1214 CA	TYR	151	25.312	43.551 101.146	1.00 19.67	HIGL HIGL
ATOM	1215 CB	TYR	151	25.949	42.403 100.362 41.515 99.711	1.00 19.65 1.00 20.60	HIĞL
ATOM	1216 CG	TYR TYR	151 151	24.910 24.183	41.962 98.610	1.00 20.83	HIGL
ATOM ATOM	1217 CD1 1218 CE1		151	23.180	41.179 98.036	1.00 20.50	HIGL
ATOM	1219 CD2		151	24.609	40.249 100.228	1.00 20.51	HIGL
ATOM	1220 CE2	TYR	151	23.601	39.457 99.656	1.00 20.06 1.00 20.06	HIGL HIGL
MOTA	1221 CZ	TYR.	151	22.894	39.933 98.559 39.171 97.972	1.00 20.00	HIGL
ATOM	1222 OH	TYR TYR	151 151	21.904 24.389	42.972 102.204	1.00 19.26	HIGL
ATOM ATOM	1223 C 1224 O	TYR	151	23.176	43.114 102.113	1.00 18.33	HIGL
ATOM	1225 N	ASN	152	24.966	42.317 103.209	1.00 19.42	HIGL
ATOM	1226 CA	ASN	152	24.158		1.00 19.11	HIGL HIGL
ATOM	1227 CB	ASN	152	25.040	41.046 105.326	1.00 19.23 1.00 20.56	HIGL
MOTA	1228 CG	ASN	152	25.663 25.221		1.00 20.36	HIGL
ATOM	1229 OD1 1230 ND2		152 152	26.687		1.00 19.90	HIGL
ATOM ATOM	1230 ND2	ASN	152	23.265	42.756 104.937	1.00 18.86	HIGL
MOTA	1232 0	ASN	152	22.111	42.469 105.248	1.00 19.25	HIGL HIGL
MOTA	1233 N	ILE	153	23.792		1.00 18.55 1.00 18.75	HIGL
ATOM	1234 CA	ILE	153	23.024	49.020 T09.004	#. 00 #01,D	

Fig. 2 cont.

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					5/174 46.283 106.033	1.00 17.77	HIGL
ATOM	1235 CB	ILE	153	23.891 23.053	46.283 106.033 47.395 106.623	1.00 16.52	HIGL
ATOM	1236 CG2 1237 CG1	ILE	153 153	25.046	45.949 106.982	1.00 17.36	HIGL
MOTA MOTA	1237 CG1	ILE	153	26.068	47.050 107.128	1.00 16.15	HIGL
ATOM	1239 C	ILE	153	21.770	45,414 105.021	1.00 19.29	HIGL
ATOM	1240 O	ILE	153	20.653		1.00 18.88 1.00 18.63	HIGL HIGL
ATOM	1241 N	ALA	154	21.950	45.791 103.758 46.198 102.936	1.00 19.02	HIGL
MOTA	1242 CA	ALA ALA	154 154	20.814 21.280	46.567 101.536	1.00 17.23	HIGL
ATOM ATOM	1243 CB 1244 C	ALA	154	19.828	45.043 102.880	1.00 19.18	HIGL
MOTA	1245 0	ALA	154	18.609	45.227 102.823	1.00 19.09	HIGL
ATOM	1246 N	ARG	155	20.393	43.846 102.908	1.00 19.15 1.00 18.74	HIGL HIGL
ATOM	1247 CA	ARG	155	19.646	42.602 102.864 41.461 102.775	1.00 18.79	HIGL
ATOM	1248 CB	ARG ARG	155 155	20.661 20.110	40.111 102.485	1.00 19.95	HIGL
ATOM ATOM	1249 CG 1250 CD	ARG	155	19.495	39.997 101.104	1.00 20.00	HIGT
ATOM	1251 NE	ARG	155 .	18.768	38.740 101.065	1.00 21.33	HIGL
ATOM	1252 CZ	ARG	155	19.341	37.554 100.901	1.00 22.66	HIGL HIGL
ATOM	1253 NH1	AŖG	155	20.655	37.462 100.728 36.454 100.981	1.00 22.62 1.00 24.41	HIGL
ATOM	1254 NH2	ARG	155 155	18.607 18.798	42.509 104.142	1.00 18.62	HIGL
ATOM ATOM	1255 C 1256 O	ARG ARG	155	17.593	42.257 104.105	1.00 18.01	HIGL
ATOM	1250 U	LEU	156	19.432	42.748 105.280	1.00 18.71	HIGL
MOTA	1258 CA	<b>LEO</b>	156	18.725	42.688 106.548	1.00 17.91	HIGL HIGL
ATOM	1259 CB	LEU	156	19.720	42.796 107.707 41.507 107.927	1.00 16.34 1.00 16.27	HIGL
MOTA	1260 CG	LEU	156 156	20.507 21.555	41.716 109.000	1.00 15.19	HIGL
ATOM ATOM	1261 CD1 1262 CD2	LEU	156	19.547	40.384 108.310	1.00 15.70	HIGL
ATOM	1262 CD2	LEU	156	17.651	43.757 106.680	1.00 17.08	HIGL
ATOM	1264 0	LEU	156	16.531	43.472 107.097	1.00 18.08	HIGL
MOTA	1265 N	LEU	157	17.984	44.987 106.323	1.00 16.61 1.00 16.27	HIGL HIGL
MOTA	1266 CA	LEU	157 157	17.025 17.710	46.069 106.448 47.405 106.169	1.00 15.39	HIGL
ATOM ATOM	1267 CB 1268 CG	LEU	157	18.901	47.674 107.103	1.00 15.27	HIGL
ATOM	1269 CD1	LEU	157	19.582	48.989 106.730	1.00 14.68	HIGL
ATOM	1270 CD2	LEU	157	18.425	47.688 108.546	1.00 13.43	HIGL HIGL
MOTA	1271 C	LEU	157	15.819	45.870 105.543 46.120 105.950	1.00 16.79 1.00 17.48	HIGL
ATOM	1272 O 1273 N	LEU HIS	157 158	14.686 16.050	45.403 104.321	1.00 17.58	HIGL
MOTA MOTA	1273 N 1274 CA	HIS	158	14.944	45.174 103.401	1.00 17.25	HIGL
ATOM	1275 CB	HIS	158	15.439	44.552 102.099	1.00 17.36	HIGL
MOTA	1276 CG	HIS	158	14.335	44.187 101.159	1.00 18.88 1.00 18.45	HIGL HIGL
ATOM	1277 CD2	HIS	158	13.798	42.986 100.834 45.133 100.484	1.00 18.45	HIGL
MOTA	1278 ND1 1279 CE1	HIS HIS	158 158	13.587 12.641	44.530 99.790	1.00 18.81	HIGL
MOTA MOTA	1280 NE2	HIS	158	12.746	43.225 99.985	1.00 19.02	HIGL
ATOM	1281 C	HIS	158	13.920	44.242 104.051	1.00 17.47	HIGL
MOTA	1282 O	HIS	158	12.723	44.531 104.066	1.00 16.46	HIGL HIGL
ATOM	1283 N	SER	159	14.402 13.535	43.127 104.592 42.157 105.244	1.00 17.53 1.00 17.96	HIGL
ATOM	1284 CA 1285 CB	SER SER	159 159	14.353	40.973 105.753	1.00 18.70	HIGL
ATOM ATOM	1286 OG	SER	159	14.963	40.280 104.684	1.00 20.45	HIGL
MOTA	1287 C	SER	159	12.778	42.782 106.409	1.00 18.11	HIGL
ATOM	1288 O	SER	159	11.577	42.549 106.577	1.00 17.79	HIGL HIGL
ATOM	1289 N	ALA	160	13.483	43.573 107.214 44.231 108.363	1.00 17.67 1.00 17.44	HIGL
MOTA	1290 CA 1291 CB	ALA ALA	160 160	12.871 13.929		1.00 16.81	HIGL
ATOM ATOM	1291 CB 1292 C	ALA	160	11.824	45.239 107.918	1.00 17.59	HIGL
ATOM	1293 0	ALA	160	10.737	45.322 108.492	1.00 17.41	HIGL
ATOM	1294 N	ALA	161	12.157	46.012 106.892	1.00 18.14	HIGL HIGL
MOTA	1295 CA	ALA	161	11.230	47.011 106.377 47.714 105.189	1.00 18.38	HIGL
ATOM	1296 CB 1297 C	ALA ALA	161 161	11.831 9.931		1.00 10.03	HIGL
MOTA MOTA	1297 C 1298 O	ALA	161	8.844		1,00 20.06	HIGL
ATOM	1299 N	TRP	162	10.045		1.00 19.98	HIGL

Fig. 2 cont.

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ATOM	1300 CA	TRP	162		8.864	44.463 104.889	1.00 20.45	HIGL
ATOM	1301 CB	TRP	162		9.215	43.511 103.746	1.00 21.00	HIGL
ATOM	1302 CG	TRP	162		9.298	44.267 102.482	1.00 21.58	HIGL
	1303 CD2	TRP	162		8.222	44.516 101.575	1.00 21.96	HIGL
MOTA	1304. CE2	TRP	162		8.691	45.440 100.612	1.00 21.86	${\tt HIGL}$
MOTA			162	•	6.902	44.056 101.487	1.00 22.03	HIGL
MOTA	1305 CE3	TRP			10.354	45.019 102.040		HIGL
ATOM	1306 CD1	TRP	162		10.334	45.729 100.919		HIGL .
MOTA	1307 NE1	TRP	162	•				HIGL
MOTA	1308 CZ2	TRP	162			45.913 99.572		HIGL
ATOM	1309 CZ3	TRP	162 ·		· 6.096	44.530 100.448	1.00 22.27	
ATOM	1310 CH2	TRP	162		6.594	45.449 99.506		HIGL
ATOM	1311 C	TRP	162		8.108	43.746 105.982	2 1.00 20.46	HIGL
MOTA	1312 0	TRP	162		6.919	43.463 105.829	9 1.00 21.30	HIGL
ATOM	1313 N	GLY	163	•	.8.783	43.453 107.085	5 1.00 19.69	$\mathtt{HIGL}$
	1314 CA	GLY	163		8.089	42.816 108.183	2 1.00 19.99	HIGL
MOTA			. 163		7 048	43.833 108.623	1.00 20.35	HIGL
MOTA	1315 C				5.954	43.491 109.07	5 1.00 20.66	HIGL
MOTA	1316 0	GLY	163 ·			45.106 108.46		HIGL
MOTA	1317 N	VAL	164		7.398	46 104 108 93		HIGL
MOTA	1318 CA .	VAL	164		6.504	46.194 108.83		HIGL
MOTA	1319 CB	VAL	164		7,266	47.534 108.94		
MOTA	1320 CG1	VAL	164		6.305	48.650 109.33		HIGL
ATOM	1321 CG2	VAL	164		8.391	47.409 109.95		HIGL
ATOM	1322 C	VAL	164		5.447	46.336 107.74		HIGL
ATOM	1323 0	VAL	164		4.254	46.415 108.02	7 1.00 18.31	HIGL
	1324 N	LYS	165		5.891	46.356 106.50		$\mathtt{HIGL}$
MOTA		LYS	165.		4.965	46.516 105.40		HIGL
MOTA	1325 CA				5.728	46.615 104.08		HIGL
ATOM	1326 CB	LYS	165	•	6.589	47.869 103.98		HIGL
MOTA	1327 CG	LYS	165					HIGL
MOTA	1328 CD	LYS	165.		7.335	47.923 102.64		HIGL
MOTA	1329 CE	LYS	165		8.175	49.182 102.53		HIGL
MOTA	1330 NZ	LYS	165		7.317	50.401 102.62		
ATOM	1331 C	LYS	165		.3.904	45.428 105.32		HIGL
ATOM	1332 O	LYS	165		2.746	45.727 105.04		HIGL
MOTA	1333 N	ASP	166		4.283	44.179 105.58	1 1.00 21.39	$\mathtt{HIGL}$
ATOM	1334 CA	ASP	166		3.327	43.073 105.52	2 1.00 22.03	HIGL
ATOM	1335 CB	ASP	166		4.039	41.749 105.21	9 1.00 22.56	HIGL
	1335 CB	ASP ·	166		4.642	41.702 103.83		HIGL
ATOM		ASP	166		4.195	42,463 102.95		HIGL
ATOM	1337 OD1		166		5.560	40.879 103.62		HIGL
MOTA	1338 OD2	ASP		-		42.860 106.78		HIGL
MOTA	1339 C	ASP ·	166		2.481	41.896 106.85		HIGL
MOTA	1340 0	ASP	166		1.724			HIGL
MOTA	1341 N	SER	167		2.596	43.732 107.77		HIGL
ATOM	1342 CA	SER	167		1.825	43.554 109.00		HIGT.
MOTA	1343 CB	SER	167		2.519	44.259 110.16		•
ATOM	1344 OG	SER	167	•	2.442	45.667 110.02		HIGL
ATOM	1345 C	SER	167		0.396	44.081 108.88		HIGL
MOTA	1346 O	SER	167		0.040	44.722 107.90	3 1.00 22.85	HIGL
ATOM	1347 N	ARG	168		-0.418	43.798 109.89	98 1.00 23.80	HIGL
	1348 CA	ARG	168		~1.805	44.250 109.93	33 1.00 23.78	HIGL
MOTA			168		-2.601	43.465 110.9		HIGL
ATOM	1349 CB	ARG			-3.597	42.463 110.43		HIGL
MOTA	1350 CG	ARG		'		41.049 110.5		$\mathtt{HIGL}$
MOTA	1351 CD	ARG	168		-3.088			HIGL
ATOM	1352 NE	ARG	168		-2.910	40.664 111.9		HIGL
ATOM	1353 CZ	ARG	168		-2.272	39.564 112.3	48 1.00 18.78	HIGL
ATOM	1354 NH1	ARG	168		-1.763	38.753 111.4	30 1.00 18.16	
ATOM	1355 NH2	ARG	168		-2.127	39.278 113.6		HIGL
ATOM	1356 C	ARG	168		-1.890	45.734 110.2	84 1.00 24.65	HIGL
ATOM	1357 0	ARG	168		-2.980	46.299 110.3	48 1.00 25.72	HIGL
	1358 N	LEU	169		-0.751	46.366 110.5	34 1.00 24.93	$\mathtt{HIGL}$
ATOM			169		-0.767	47.779 110.8		HIGL
MOTA	1359 CA	ĽEU			0.642	48.300 111.1		HIGL
ATOM	1360 CB	LEU	169	•		47.981 112.5		HIGL
ATOM	1361 CG	LEU	169		1.239	47.301 114.3		HIGL
ATOM	1362 CD1		169		2.643	48.570 112.5		HIGL
ATOM	1363 CD2		169		0.350	48.545 113.5		HIGL
MOTA	1364 C	LEU	169		-1.395	48.596 109.7	68 1.00 26.78	nigh

Fig. 2 cont.

ATOM

# 67/174 1.00 26.61 HIGL 48.421 108.591 -1.086 169 LEU 1365 O ATOM HIGL 49.485 110.160 1.00 28.98 -2.292 170 1366 N ASN ATOM 1.00 31.16 HIGL 50.356 109.216 -2.962 170 ASN 1367 CA ATOM HIGL 49.638 108.536 1.00 34.31 170 -4.126 1368 CB ASN ATOM 1.00 37.73 HIGL 50.301 107.223 -4.532170 1369 CG ASN ATOM 50.087 106.717 1.00 39.55 HIGL -5.637 170 1370 OD1 ASN ATOM 51.098 106.657 HIGL 1.00 38.83 -3.628 170 1371 ND2 ASN ATOM HIGL 51.560 109.989 1.00 31.18 -3.482 170 MOTA 1372 C ASN 51.411 110.965 1.00 31.87 HIGL -4.227 -3.044 -3.373 1373 O 170 ASN ATOM 1.00 29.94 HIGL 52.767 109.599 171 MOTA 1374 N PRO HIGL 1.00 29.80 54.060 110.227 1375 CD PRO 171 ATOM 1.00 28.18 1.00 28.38 HIGL -2.101 -2.094 52.949 108.492 171 MOTA 1376 CA PRO HIGL 54,459 108.295 171 1377 CB PRO MOTA 1.00 29.83 HIGL -2.269 -0.728 54.960 109.698 171 137B CG PRO MOTA 1.00 26.71 HIGL 52.413 108.889 171 PRO ATOM 1379 C HIGL 1.00 25.16 -0.472 52.183 110.068 171 PRO MOTA 1380 O 52:204 107.900 1.00 25.19 HIGL 172 0.139 LYS MOTA 1381 N HIGL 1.00 24.35 1.482 51.709 108.155 172 1382 CA LYS MOTA 51.187 106.867 1.00 25.60 HIGL 2.119 1383 CB 172 LYS ATOM 1.00 27.94 .HIGL 1.274 50.201 106.093 172 1384 CG LYS MOTA 1.00 29.37 48.826 106.725 HIGL 1.253 1385 CD LYS 172 ATOM 1.00 30.03 · HIGL 47.875 105.848 0.451 172 LYS 1386 CE MOTA 46.469 106.329 HIGL 1.00 30.93 0.492 172 LYS ATOM 1387 NZ HIGL 1.00 22.94 52.858 108.686 2.332 1388 C 172 MOTA LYS 53.992 108.220 HIGL 1.00 22.83 172 2.212 1389 O LYS MOTA HIGL 3.200 1.00 21.18 52.580 109.671 ATOM 173 1390 N PRO 1:00 21.36 HIGL 51.290 110.354 173 3.396 1391 CD PRO ATOM 1.00 20.28 HIGL 53.599 110.254 4.069 173 1392 CA PRO MOTA 1.00 20.26 1.00 20.58 HIGL 52.915 111.508 173 4.595 PRO ATOM 1393 CB HIGL 51.502 111.059 4.718 1394 CG PRO 173 MOTA 53.947 109.297 1.00 19.51 HIGL 173 173 5.197 PRO ATOM 1395 C 1.00 19.40 HIGL 53.172 108.407 5.525 ATOM PRO 1396 O 1.00 18.84 HIGL 55.123 109.482 174 174 5.778 LYS 1397 N ATOM 1.00 18.05 HIGL 6.887 55.548 108.655 LYS ATOM 1398 CA HIGL 57.032 108.875 1.00 18.15 174 174 7.168 LYS 1399 CB ATOM 1.00 18.80 HIGL 57.905 108.527 5.984 ATOM 1400 CG LYS 1.00 19.52 1.00 18.38 HIGL 59.380 108.602 174 6.308 LYS MOTA 1401 CD 60.200 108.085 HIGL 5.140 174 ATOM 1402 CE LYS 1.00 19.70 HIGL 61.622 107.893 174 5.521 LYS 1403 NZ MOTA HIGL 1.00 17.68 54.712 109.097 8.073 174 MOTA 1404 C LYS 1.00 18.33 1.00 17.03 HIGL 54.586 110.288 174 8.348 LYS MOTA 1405 O HIGL 54.119 108.139 8.764 175 ILE MOTA 1406 N 1.00 16.37 HIGL 53.291 108.461 ILE 175 9.909 1407 CA MOTA HIGL 10.071 52.178 107.420 1.00 15.88 ATOM 175 1408 CB ILE 1.00 14.85 HIGL 175 11.276 51.317 107.767 ILE MOTA 1409 CG2 HIGL 1.00 14.92 51.342 107.387 8.785 175 1410 CG1 ILE MOTA 1.00 16.47 50.358 106.232 HIGL 8.694 ILE 175 MOTA 1411 CD1 HIGL 54.176 108.517 1.00 15.73 11.142 175 MOTA 1412 C ILE 1.00 15.78 HIGL 54.933 107.588 175 11.417 ILE **ATOM** 1413 O HIGL 1.00 14.73 54.075 109.620 11.874 ATOM MET 176 1414 N 1.00 14.35 HIGL 54.896 109.836 176 13.054 MET ATOM 1415 CA HIGL 12.830 55.786 111.070 1.00 13.52 176 176 MET 1416 CB ATOM 1.00 13.16 HIGL 56.557 111.518 14.060 MET MOTA 1417 CG 1.00 14.72 1.00 14.08 HIGL 13.928 57.167 113.201 176 1418 SD MET MOTA HIGL 12.695 14.358 58.477 112.999 176 1419 CE MET ATOM HIGL 54.122 110.024 1.00 14.18 176 1420 C MET ATOM HIGL 53.040 110.603 1.00 14.19 176 14.376 1421 O MET ATOM 54.693 109.511 HIGL 15.444 16.777 17.532 1.00 14.60 177 1422 N VAL MOTA 1.00 13.89 HIGL 54.123 109.664 177 MOTA 1423 CA VAL HIGL 54.024 108.319 1.00 13.58 177 VAL 1424 CB ATOM HIGL 1.00 12.32 177 19.004 53.680 108.573 ATOM 1425 CG1 VAL HIGL 52.940 107.454 1.00 12.15 177 16.892 1426 CG2 VAL MOTA HIGL 17.461 55.113 110.597 1.00 13.92 177 MOTA 1427 C VAL 1.00 13.57 HIGL 56.314 110.326 177 17.503 VAL 1428 O MOTA 1.00 14.28 54.595 111.710 17.966 1429 N HIS 178

Fig. 2 cont.

ATOM

MOTA

MOTA

ATOM

MOTA

MOTA

MOTA

MOTA

MOTA

MOTA

ATOM

1484 CG

1485 OD1

1486 ND2

1487 C

1488 O

1489 N

1490 CA

1491 CB

1492 CG

1493 CD2

1494 CE2

ASN

ASN

ASN

ASN

ASN

TRP

TRP

TRP

TRP

TRP

TRP

184

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# 68/174 178 18.591 55.407 112.743 1.00 14.37 HIGL HIS ATOM 1430 CA 1.00 14.38 1.00 14.85 55.083 114.083 HIGL 178 17.910 ATOM 1431 CB HIS 18.522 55.762 115.268 18.456 55.471 116.589 178 HIGL MOTA 1432 CG HIS 1.00 14.94 HIGL 178 MOTA 1433 CD2 HIS 19.287 1.00 15.06 178 56.903 115.163 HIGL ATOM 1434 ND1 HIS 57.285 116.369 56.434 117.251 55.235 112.850 1.00 14.39 HIGL 1435 CE1 178 19.670 ATOM HIS 178: 19.179 1.00 15.19 HIGL ATOM 1436 NE2 HIS 1.00 14.74 HIGL 178 20.102 MOTA HIS 1437 C 178 179 1.00 14.60 54.132 113.072 HIGL 20.605 ATOM 1438 O HIS 1.00 14.60 1.00 14.68 1.00 14.85 1.00 15.01 1.00 15.16 1.00 14.52 56.346 112.685 56.381 112.769 56.817 111.430 HIGL 20.812 ATOM 1439 N LEU LEU 179 22.269 HIGL MOTA 1440 CA HIGL 179 LEU 22.866 MOTA 1441 CB 179 179 55.794 110.349 54.786 110.177 23.217 HIGL 1442 CG LEU MOTA 22.120 HIGL 1443 CD1 LEU ATOM . 56.536 109.049 57.406 113.830 179 23.476 HIGL LEU ATOM 1444 CD2 HIGL 179 22.632 1.00 14.77 1.00 16.15 1.00 14.56 1.00 15.13 1.00 15.21 1.00 16.64 1.00 15.02 1.00 16.16 1.00 15.95 1.00 17.25 1.00 15.67 1.00 16.57 1.00 17.66 1.00 19.18 MOTA 1445 C LEU 179 21.867 58.336 114.070 HIGL LEU MOTA 1446 O 23.786 HIGL 180 57.244 114.468 MOTA 1447 N ASP 24.217 58.200 115.483 57.491 116.576 180 HIGL 1448 CA ASP ATOM HIGL 1449 CB ASP 180 ATOM 57.238 116.171 56.712 115.060 26.496 HIGL 1450 CG ASP 180 ATOM 26.744 27.393 25.039 HIGL ATOM 1451 OD1 ASP 180 57.560 116.987 59.279 114.776 180 HIGL 1452 OD2 ASP ATOM ASP . 180 HIGL MOTA 1453 C 180 25.185 59.233 113.555 HIGL 1454 O ASP ATOM 25.556 26.362 27.754 60.249 115.525 HIGL ASŃ 181 ATOM 1455 N 181 61.334 114.960 HIGL MOTA 1456 CA NZA 60.824 114.594 HIGL 181 ATOM 1457 CB ASN 26.573 28.418 181 HIGL 1458 CG ASN 60.449 115.807 MOTA 1.00 19.18 1.00 18.44 61.031 116.881 HIGL ATOM 1459 OD1 ASN 181 29.464 25.763 59.487 115.641 HIGL ATOM 1460 ND2 ASN 181 1.00 15.63 1.00 15.55 1.00 15.79 1.00 15.12 62.034 113.742 HIGL 181 1461 C MOTA ASN 26.433 24.508 HIGL 62.200 112.731 ATOM 1462 O ASN 181 1463 N 182 62.455 113.847 HIGL GLY MOTA 63.129 112.744 64.373 112.287 1464 CA 1465 C HIGL GLY 182 23.853 ATOM 1.00 15.79 1.00 16.16 182 24.575 HIGL GLY ATOM 24.331 25.459 26.227 HIGL 182 1466 O GLY 64.857 111.184 MOTA 1.00 16.94 1.00 16.80 64.902 113.130 66.100 112.784 183 HIGL ATOM 1467 N TRP .183 183 HIGL ATOM 1468 CA TRP 26.854 27.735 1.00 16.19 1.00 14.99 1469 CB 66.746 114.034 HIGL TRP MOTA HIGL 183 65.829 114.837 ATOM 1470 CG TRP 1471 CD2 1472 CE2 65.506 114.577 64.558 115.547 1.00 14.85 1.00 14.72 183 29.108 HIGL ATOM TRP HIGL 29.505 ATOM TRP 183 30.041 27.369 1.00 15.26 1.00 15.04 1473 CE3 183 . 65.922 113.616 HIGL TRP ATOM 65.091 115.919 64.324 116.353 64.015 115.586 HIGL MOTA 1474 CD1 TRP 183 28.424 30.798 1475 NE1 183 1.00 14.56 HIGL ATOM TRP 1.00 13.96 HIGL 1476 CZ2 183 ATOM TRP 1.00 14.45 HIGL 1477 CZ3 183 31.332 65.379 113.654 MOTA TRP 31.332 31.693 27.333 27.780 27.780 28.838 29.623 30.892 1.00 13.99 HIGL 1478 CH2 183 64.436 114.634 ATOM TRP 65.755 111.797 66.606 111.040 1.00 17.18 1.00 18.90 HIGL 183 ATOM 1479 C TRP HIGL ATOM 1480 O TRP 183 1.00 17.37 1481 N 64.508 111.807 HIGL 184 ATOM ASN 64.087 110.901 1.00 18.52 HIGL MOTA 1482 CA NZA 184 1483 CB 62.936 111.514 62.651 110.760 ATOM ASN 184 1.00 18.43 HIGL

Fig. 2 cont.

62.652 109.528

62.403 111.490

63.647 109.551

62.515 109.406

64.536 108.563

64.239 107.246

65.517 106.404

65.269 104.923

64.623 104.224

64.564 102.857

30.904

31.972

28.265 27.800

28.318 27.780

27.752

27.658

26.584 26.952

1.00 18.15

1.00 17.65

1.00 16.66

1.00 19.20

1.00 19.59

1.00 18.87

1.00 18.50

1.00 19.66

1.00 20.74

1.00 21.65

1.00 21.97

HIGL

100 10.0	·				
				69/174	
ATOM	1495 CE3	TRP	185	25.349 64.085 104.618 1.00 21.22	HIGL HIGL
MOTA	1496 CD1	TRP	185	28.601 65.570 103.982 1.00 20.45 28.184 65.151 102.740 1.00 21.70	HIGL
MOTA	1497 NE1	TRP	185	28.184 65.151 102.740 1.00 21.70 26.127 63.985 101.880 1.00 21.82	HIGL
MOTA	1498 CZ2 1499 CZ3	TRP TRP	185 185	24.526 63.509 103.645 1.00 21.31	HIGL
ATOM ATOM	1500 CH2	TRP	185	24.921 63.465 102.292 1.00 21.28	HIGL
MOTA	1501 C	TRP	185	28.510 63.126 106.489 1.00 18.87	HIGL HIGL
ATOM	1502 0	TRP	185	27.873 62.328 105.796 1.00 18.21 29.835 63.074 106.606 1.00 18.26	HIGL
MOTA	1503 N	ASP	186 186	29.835 63.074 106.606 1.00 18.26 30.595 62.042 105.918 1.00 18.41	HIGL
ATOM ATOM	1504 CA 1505 CB	ASP ASP	186	32.094 62.185 106.181 1.00 19.07	HIGL
MOTA	1506 CG	ASP	186	32.662 63.492 105.644 1.00 19.86	HIGL
ATOM	1507 OD1	ASP	186	32.235 63.922 104.546 1.00 18.31 33.539 64.082 106.321 1.00 20.67	HIGL HIGL
MOTA	1508 OD2	ASP	186	33.539 64.082 106.321 1.00 20.67 30.127 60.669 106.375 1.00 18.79	HIGL
ATOM	1509 C 1510 O	ASP ASP	186 186	30.057 59.738 105.569 1.00 19.44	HIGL
MOTA MOTA	1511 N	THR	187	29.804 60.541 107.662 1.00 18.54	HIGL
ATOM	1512 CA	THR	187	29.326 59.267 108.185 1.00 18.36 29.144 59.303 109.717 1.00 18.81	HIGL HIGL
ATOM	1513 CB	THR	187	200 17 30	HIGL
ATOM	1514 OG1	THR	187 [.] 187	30.334 59.779 110.359 1.00 17.18 28.841 57.898 110.229 1.00 17.29	HIGL
MOTA MOTA	1515 CG2 1516 C	THR THR	187	27.955 58.970 107.554 1.00 18.81	HIGL
ATOM	1517 0	THR	187	27.749 57.924 106.953 1.00 18.82	HIGL HIGL
ATOM	1518 N	GLN	188	27.028 59.912 107.690 1.00 18.92 25.678 59.756 107.123 1.00 18.70	HIGL
ATOM	1519 CA	GLN	188 188	25.678 59.756 107.123 1.00 18.70 24.868 61.025 107.278 1.00 18.92	HIGL
ATOM ATOM	1520 CB 1521 CG	GLN GLN	188	24 691 61.548 108.719 1.00 20.75	HIGL
MOTA	1522 CD	GLN	188	24.217 60.494 109.715 1.00 21.45	HIGL
MOTA	1523 OE1	GLN	188	23.340 59.658 109.425 1.00 21.55 24.775 60.558 110.916 1.00 20.88	HIGL HIGL
ATOM	1524 NE2	GLN	188	24.775 60.558 110.916 1.00 20.88 25.693 59.419 105.628 1.00 18.27	HIGL
MOTA	1525 C 1526 O	GLN GLN	188 188	24.854 58.643 105.144 1.00 19.06	HIGL
ATOM ATOM	1527 N	ASN	189	26,652 60.019 104.912 1.00 18.01	HIGL
ATOM	1528 CA	ASN	189	26.837 59.855 103.466 1.00 17.83 27.713 61.007 102.897 1.00 18.12	HIGL
ATOM	1529 CB	ASN	189	27.713 61.007 102.897 1.00 18.12 27.816 60.975 101.367 1.00 18.97	HIGL
ATOM ATOM	1530 CG 1531 OD1	ASN ASN	189 189	27.022 60.302 100.708 1.00 18.06	HIGL
ATOM	1532 ND2	ASN	189	28.776 61.718 100.800 1.00 19.12	HIGL
MOTA	1533 C	ASN	189	27.460 58.493 103.165 1.00 17.73 26.935 57.760 102.331 1.00 17.69	HIGL HIGL
MOTA	1534 0	ASN	189 190	26.935 57.760 102.331 1.00 17.69 28.583 58.180 103.812 1.00 17.17	HIGL
MOTA MOTA	1535 N 1536 CA	TRP TRP	190	29.272 56.895 103.656 1.00 16.53	HIGL
MOTA	1537 CB	TRP	190	30.409 56.855 104.679 1.00 16.92	HIGL
MOTA	1538 CG	TRP	190	30.943 55.516 105.033 1.00 17.78 30.714 54.794 106.253 1.00 17.06	HIGL
ATOM	1539 CD2	TRP	190	30.714 54.794 106.253 1.00 17.06 31.490 53.620 106.192 1.00 18.29	HIGL
MOTA MOTA	1540 CE2 1541 CE3	TRP TRP	190 190	29.931 55.028 107.392 1.00 17.68	HIGL
ATOM	1542 CD1		190	31.811 54.770 104.303 1.00 18.04	HIGL
MOTA	1543 NE1	TRP	190	32.150 53.630 104.991 1.00 18.09 31.511 52.675 107.230 1.00 18.43	HIGL HIGL
ATOM	1544 CZ2		190 190	31.511 52.675 107.230 1.00 18.43 29.951 54.083 108.431 1.00 18.02	HIGL
MOTA MOTA	1545 CZ3 1546 CH2		190	30.738 52.925 108.336 1.00 17.37	HIGL
ATOM	1547 C	TRP	190	28.307 55.715 103.874 1.00 15.60	HIGL
ATOM	1548 O	TRP	190	28.193 54.800 103.053 1.00 16.16 27.609 55.744 104.997 1.00 14.48	HIGL
ATOM	1549 N	TRP	191	27.609 55.744 104.997 1.00 14.48 26.674 54.686 105.327 1.00 14.21	HIGL
MOTA	1550 CA 1551 CB	TRP TRP	191 191	26.028 54.956 106.681 1.00 12.41	HIGL
ATOM ATOM	1552 CG	TRP	191	25.437 53.729 107.273 1.00 11.51	HIGL
ATOM	1553 CD2	TRP	191	24,101 53.250 107.097 1.00 10.28	HIGL HIGL
ATOM	1554 CE2		191	23.990 52.044 107.827 1.00 10.64 22.986 53.720 106.393 1.00 7.88	HIGL
MOTA	1555 CE3 1556 CD1		191 191	22.986 53.720 106.393 1.00 7.88 26.068 52.820 108.074 1.00 12.10	HIGL
ATOM ATOM	1556 CD1		191	25,208 51.805 108.413 1.00 10.86	HIGL
ATOM	1558 CZ2	TRP	191 .	22.808 51.304 107.876 1.00 9.13	HIGL HIGL
ATOM	1559 CZ3		191	21.818 52.988 106.440 1.00 8.78	111011

Fig. 2 cont.

				70	)/174			
ATOM	1560 CH2	TRP	191 [.]	21.735	51.790 1		1.00 9.52	HIGL
MOTA	1561 C	TRP	191	25.566	54.471 1		1.00 14.99	HIGL
ATOM	1562 0	TRP	191	25.485	53.409		1.00 14.62 1.00 15.56	HIGL HIGL
ATOM		TYR	192	24.703	55.468		1.00 15.50	HIGL
MOTA	1564 CA	TYR	192	23.595	55.341 5 56.615	103.170	1.00 15.03	HIGL
ATOM	1565 CB	TYR	192 192	22.739 21.859	56.737	104.428	1.00 14.42	HIGL
ATOM	1566 CG 1567 CD1	TYR	192	20.759	55.886	104.617	1.00 14.00	HIGL
ATOM ATOM	1568 CE1	TYR	192	19.954	55.987	105.746	1.00 13.21	HIGL
ATOM	1569 CD2	TYR	192	22.128	57.691	105.408	1.00 13.33	HIGL
MOTA	1570 CE2	TYR	192	21.332	57.804	106.544	1.00 13.35 1.00 13.89	HIGL HIGL
MOTA	1571 CZ	TYR	192	20.244	56.950 57.073	106.709	1.00 13.69	HIGL
MOTA	1572 OH	TYR	192	19.442 24.052	55.015	101.760	1.00 17.04	HIGL
ATOM	1573 C	TYR TYR	192 192	23.433	54.199	101.071	1.00 17.52	HIGL
ATOM ATOM	1574 O 1575 N	THR	193	25.137	55.643	101.325	1.00 17.90	HIGL
ATOM	1576 CA	THR	193	25.654	55.388	99.993	1.00 18.57	HIGL
ATOM	1577 CB	THR	193	26.949	56.186	99.738	1.00 19.70	HIGL
ATOM	1578 OG1	THR	193	26.634	57.582	99.645	1.00 20.25	HIGL HIGL
ATOM	1579 CG2	THR	193	27.629	55.716	98.441 99.842	1.00 17.66 1.00 18.55	HIGL
ATOM	1580 C	THR	193	25.950 25.442	53.897 53.230	98.937	1.00 18.73	HIGL
MOTA	1581 O 1582 N	THR ASN	193 194	26.772	53.230	100.742	1.00 17.82	HIGL
MOTA MOTA	1583 CA	ASN	194	27.127	51,972	100.693	1.00 18.02	HIGL
ATOM	1584 CB	ASN	194	28.166	51.663	101.762	1.00 17.18	HIGL
ATOM	1585 CG	ASN	194	29.546	52.148	101.381	1.00 16.79	HIGL
ATOM	1586 OD1			30.135		100.411	1.00 17.28 1.00 16.49	HIGL HIGL
ATOM	1587 ND2	ASN	194	30.073		102.137	1.00 18.45	HIGL
ATOM	1588 C	ASN	194	25.934 25.860		100.123	1.00 20.21	HIGL
MOTA	1589 O 1590 N	ASN VAL	194 195	25,003	51.345	101.724	1.00 17.31	HIGL
ATOM ATOM	1590 N 1591 CA	VAL	195	23.838		101.908	1.00 17.12	HIGL
MOTA	1592 CB	VAL	195	23.052		103.185	1.00 17.17	HIGL
MOTA	1593 CG1	VAL	195	21.789		103.290	1.00 16.39 1.00 16.35	HIGL KIGL
MOTA	1594 CG2	VAL	195	23.906		104.411 100.711	1.00 18.33	HIGL
MOTA	1595 C	VAL	195 195	22.882 22.414	49 514	100.711	1,00 17,57	HIGL
MOTA	1596 O 1597 N	VAL LEU	195	22.591	51.755	100.234	1.00 17.80	HIGL
ATOM ATOM	1598 CA	LEU	196	21.672	51.906	99.114	1.00 18.71	HIGL
ATOM	1599 CB	LEU	196	21.164	53.346	99.049	1.00 19.05	HIGL
ATOM	1600 CG	LEU	196	20.389		100.284	1.00 19.84	HIGL HIGL
MOTA	1601 CD1	LEU	196	19.935	55.255		1.00 19.18 1.00 18.91	HIGL
MOTA	1602 CD2		196	19.188 22.219	52.901	100.532 97.745	1.00 18.86	HIGL
MOTA	1603 C 1604 O	LEU LEU	196 196	21.446	51.326		1.00 18.34	HIGL
MOTA MOTA	1605 N	SER	197	23.537	51.316	97.631	1.00 18.55	HIGL
ATOM	1606 CA	SER	197	24.126			1.00 18.26	HIGL
ATOM	1607 CB	SER	197	25.561			1.00 17.73	HIGL HIGL
MOTA	1608 OG	SER	197	26.436			1.00 18.32 1.00 18.38	HIGL
ATOM	1609 C	SER	197	24.113 24.322			1.00 18.33	HIGL
ATOM	1610 0	SER	197 198	23.859			1.00 18.80	HIGL
MOTA MOTA	1611 N 1612 CA	GLN GLN	198	23.822			1.00 18.22	HIGL
ATOM	1613 CB	GLN	198	23.686		98.620	1.00 19.28	HIGL
ATOM	1614 CG	GLN	198	24.836			1.00 19.81	HIGL
MOTA	1615 CD	GLN	198	26.161			1.00 21.32	HIGL HIGL
MOTA	1616 OE1		198	26.353			1.00 21.68 1.00 21.99	HIGL
ATOM	1617 NE2		198	27.091			1.00 21.99	HIGL
MOTA	1618 C	GLN	198 198	22.682 22.877				HIGL
ATOM ATOM	1619 O 1620 N	GLN GLY	198	21.486			1.00 17.03	. HIGL
MOTA	1621 CA	GLY	199	20.347			1.00 15.62	HIGL
MOTA	1622 C	GLY	199	19.181	46.278			HIGL
MOTA	1623 O	GLY	199	18.045				HIGL HIGL
MOTA	1624 N	PRO	200	19.422	45.336	5 97.488	1.00 15.34	UTGL
				-		4		

Fig. 2 cont.

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ATOM ATOM	1625 CD 1626 CA	PRO PRO	200 200	20.704 44.672 97.78 18.350 44.764 98.30	6 1.00 14.92 H	IGL IGL
ATOM	1627 CB	PRO	200	19.104 43.814 99.22		IGL . IGF
ATOM	1628 CG	PRO	200	20.245 43.367 98.36 17.518 45.794 99.07		IGL
MOTA	1629 C .	PRO	200			IGL
ATOM	1630 0	PRO	200	16.288 45.699 99.11 18.178 46.771 99.69		IGL
ATOM	1631 N	PHE	201 201	17.457 47.806 100.43	9 1.00 17.91 H	IGL
MOTA	1632 CA 1633 CB	PHE PHE	201	18 296 48.317 101.60	7 1.00 17.39 H	IGL
MOTA MOTA	1634 CG	PHE	201	17.523 49.154 102.58	2 T100 T11-	IGL
ATOM	1635 CD1	PHE	201	16.320 48.696 103.10		IGL IGL
ATOM	1636 CD2 .	PHE	201	18.019 50.376 103.01 15.627 49.436 104.04		IGL .
MOTA	1637 CE1	PHE	201	15.627 49.436 104.04 17.331 51.130 103.96	2.00 ~	IGL
ATOM	1638 CE2 1639 CZ	PHE PHE	201 201	16.133 50.658 104.48	34 1.00 16.02 H	HIGL .
ATOM ATOM	1640 C	PHE	201	17.160 48.947 99.48	31 1.00 19.32 H	IIGL
ATOM .	1641 0	PHE	201	18.052 49.707 99.11		RIGL
ATOM	1642 N	GLU	202	15.899 49.066 99.08	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	HIGL HIGL
ATOM	1643 CA	GLU	202	15.492 50.079 98.13 14.381 49.527 97.24		HIGL
ATOM		GLU	202	14.381 49.527 97.26 14.646 48.127 96.73	10 1100 201	HIGL
ATOM	1645 CG 1646 CD	GLU GLU	202 202	13.649 47.709 95.6	70 1.00 31.92 F	HIGL
ATOM ATOM	1647 OE1	GLU	202	13,642 48.342 94.5	88 1.00 33-85 I	HIGL
ATOM	1648 OE2	GLU	202	12.876 46.758 95.9	10 1100 001	HIGL HIGL
MOTA	1649 C	GLU	202	15.033 51.394 98.7 14.660 51.473 99.8		HIGL
MOTA	1650 O	GLU	202	14.660 51.473 99.8 15.046 52.426 97.8	J2 1.00 LL.	HIGL
ATOM	1651 N 1652 CA	MET MET	203 203	14.624 53.748 98.3	09 · 1.00 23.40	HIGL
ATOM ATOM	1653 CB	MET	203	14.768 54.734 97.1	JJ +100	HIGL
MOTA	1654 CG		. 203	16.202 55.007 96.7	0, 1.00 2, 0	HIGL HIGL
MOTA	1655 SD	MET	203	17.161 55.583 98.1 16.411 57.199 98.4	75 1.00 00.00	HIGL
ATOM	1656 CE	MET	203 203	16.411 57.199 98.4 13.185 53.748 98.8	· · · · · · · · · · · · · · · · · · ·	HIGL
ATOM ATOM	1657 C 1658 O	MET MET	203	12.835 54.522 99.6	96 1.00 22.95	HIGL
MOTA	1659 N	SER	204	12.352 52.878 98.2		HIGL HIGL
ATOM	1660 CA	SER	204	10.956 52.823 98.6 10.077 52.307 97.5	700 1.00 22	HIGL
MOTA	1661 CB	SER	204	10.077 52.307 97.5 10.458 51.006 97.1	21 1.00 11	HIGL
ATOM	1662 OG 1663 C	SER SER	204 204	10.741 51.961 99.9	13 1.00 21.58	HIGL
MOTA MOTA	1664 O	SER	204	9.610 51.822 100.3	1.00 21.09	HIGL ·
ATOM	1665 N	ASP	205	11.821 51.388 100.4	148 1.00 20.89 540 1.00 20.32	HIGL HIGL
ATOM	1666 CA	ASP	205	11.723 50.545 101.6 12.882 49.539 101.		HIGL
MOTA	1667 CB	ASP ASP	205 205	12.882 49.539 101.7 12.750 48.411 100.		HIGL
ATOM ATOM	1668 CG 1669 OD1		205	11.607 47.992 100.4	424 1.00 20.12	HIGL
ATOM	1670 OD2		205	13.792 47.933 100.	220 1.00 19.93	HIGL HIGL
ATOM	1671 C	ASP	205	11.681 51.325 102.	944 1.00 19.69 971 1.00 19.83	HIGL
MOTA	1672 0	ASP	205	11.284 50.780 103. 12.109 52.584 102.		HIGL
ATOM	1673 N	PHE PHE	206 206	12.062 53.377 104.	149 1.00 19.43	HIGL
ATOM ATOM	1674 CA 1675 CB	PHE	206	13.413 53.376 104.	877 1.00 19.75	HIGL
MOTA	1676 CG	PHE	206	14.492 54.155 104.	194 1.00 20.11	HIGL HIGL
ATOM	1677 CD1		206	14.975 53.768 102.	951 1.00 20.98 839 1.00 19.93	HIGL
ATOM	1678 CD2		206	15.090 55.233 104. 16.048 54.442 102.		HIGL
MOTA	1679 CE1 1680 CE2		206 206	16.154 55.908 104.	264 1.00 19.23	HIGL
MOTA MOTA	1681 CZ	PHE	206	16.636 55.509 103.	025 1.00 19.95	HIGL
MOTA	1682 C	PHE	206	11.588 54.791 103.	900 1.00 19.04	HIGL HIGL
ATOM		PHE	206	11.597 55.267 102. 11.173 55.462 104.	773 1.00 19.32 965 1.00 19.22	HIGL
MOTA		ASP	207	11.173 55.462 104. 10.636 56.810 104.		HIGL
ATOM		ASP ASP	207 207	9.175 56.802 105.	286 1.00 19.16	HIGL
ATOM ATOM		ASP	207	8,407 55.625 104.	718 1.00 19.38	HIGL
MOTA			207	8.277 55.543 103.	480 1.00 20.06	HIGL HIGL
ATOM			207	7.942 54.778 105.	507 1.00 18.36	117.41

7.942 54.778 105.50 Fig. 2 cont.

					1474		
					2/174	1.00 18.86	HIGL
ATOM	1690 C	ASP	207	11.381 11.381		1.00 19.26	HIGL
ATOM	1691 0	ASP	207 208	12.015		1.00 18.21	HIGL
ATOM	1692 N 1693 CA	MET MET	208	12.714	58.433 107.540	1.00 18.11	HIGL
MOTA MOTA	1693 CA 1694 CB	MET	206	12.006	58.596 108.894	1.00 18.41	HIGL
ATOM	1695 CG	MET	208	10.534	58.987 108.820	1.00 20.52	${\tt HIGL}$
ATOM	1696 SD	MET .	208	9.808	59.310 110.452	1.00 22.01	HIGL
MOTA	1697 CE	MET	208	10.379	60.977 110.731	1.00 20.87	HIGL
ATOM	1698 C .	MET	208	14.161	58.083 107.804	1.00 17.69 1.00 17.61	HIGL HIGL
MOTA	1699 0	MET	208	14.579	56.928 107.707 59.119 108.129	1.00 16.92	HIGL
MOTA	1700 N	met Met	209 209	14.918 16.308	58.994 108.488	1.00 16.07	HIGL
ATOM ATOM	1701 CA 1702 CB	MET	209	17.213	59.645 107.443	1.00 16.00	HIGL
MOTA	1702 CB	MET .	209	17.373	58.828 106.170	1.00 16.81	HIGL
ATOM	1704 SD	MET	209	18.554	59.575 105.009	1.00 19.85	HIGL
ATOM	1705 CE	MET	209	18.496	58.407 103.621	1.00 17.63	HIGL
ATOM	1706 C	MET	209	16374	59.747 109.809	1.00 16.16	HIGL HIGL
ATOM	1707 0	MET .	209	16.174	60.969 109.850 59.001 110.891	1.00 15.45 1.00 15.65	HIGL
ATOM	1708 N	GLY	210 210	16.600 16.695	59.603 112.210	1.00 14.42	HIGL
ATOM.	1709 CA. 1710 C	GLY	210	18.150	59.686 112.629	1.00 14.08	HIGL
MOTA MOTA	1711 0	GLY	210	18.961	58.883 112.175	1.00 13.68	HIGL
ATOM	1712 N	VAL	211	18.490	60.651 113.484	1.00 13.61	HIGL
MOTA	1713 CA	JAV	211	19.869	60.802 113.936	1.00 13.15	
ATOM	1714 CB	VAL	211	20.627	61.892 113.141	1.00 12.33	HIGL
MOTA	1715 CG1	VAL	211	20.537	61.611 111.663 63.271 113.465	1.00 13.18 1.00 11.20	HIGL
MOTA	1716 CG2	VAL.	211 _. 211	20.067 19.984	61.175 115.400	1.00 13.77	· HIGL
ATOM ATOM	1717 C 1718 O	VAL VAL	211	19.118	61.837 115.958	1.00 13.69	· HIGL
MOTA	1718 U	SER	212	21.069	60.741 116.022	1.00 15.09	HIGL
ATOM	1720 CA	SER	212		61.079 117.411	1.00 15.93	HIGL
ATOM	1721 CB	SER	212	22.016	59,929 118.130	1.00 16.46	HIGL
ATOM	1722 OG	SER	212	21.185	58.781 118.176	1.00 17.21 1.00 16.32	HIGL HIGL
ATOM	1723 C	SER	212	22.208 23.149	62.315 117.376 62.395 116.582	1.00 16.32	HIGL
MOTA	1724 O 1725 N	SER PHE	212 213	23.149	63.289 118.214	1.00 15.23	HIGL
MOTA MOTA	1725 N 1726 CA	PHE	213	22.666	64.512 118.267	1.00 15.45	HIGL
ATOM	1727 CB	PHE	213	21.923	65.634 117.528	1.00 15.73	HIGL
ATOM	1728 CG	PHE	213	22.673	66.936 117.484	1.00 16.40	HIGL
MOTA	1729 CD1	PHE	.213	23.883	67.036 116.799	1.00 16.45	$\mathtt{HIGL}$
MOTA	1730 CD2	PHE	213	22.183	68.057 118.146 68.231 116.777	1.00 16.56 1.00 15.36	HIGL
ATOM	1731 CE1 1732 CE2	PHE PHE	213 213	24.596 22.889	69.257 118.130	1.00 16.74	HIGL
MOTA MOTA	1732 CE2	PHE	213	24.100	69.340 117.443	1.00 16.06	HIGL
ATOM	1734 C	PHE	213	22.849	64.850 119.738	1.00 14.96	HIGL
MOTA	1735 0	PHE	213	21.888	65.175 120.436	1.00 15.30	HIGL
MOTA	1736 N	TYR	214	24.085	64.742 120.208	1.00 14.20	HIGL HIGL
MOTA	1737 CA	TYR	214	24.420	65.016 121.600	1.00 13.58 1.00 12.69	HIGL
MOTA	1738 CB	TYR	214	24.875 23.775	63.736 122.298 62.742 122.558	1.00 12.09	HIGL
MOTA	1739 CG 1740 CD1	TYR TYR	214 214	22.902	62.906 123.631	1.00 11.71	HIGL
ATOM ATOM	1740 CE1	TYR	214	21.885	61.989 123.874	1.00 11.65	HIGL
ATOM	1742 CD2	TYR	214	23.602	61.635 121.731	1.00 10.99	HIGL
ATOM	1743 CE2	TYR	214	22.591	60.717 121.962	1.00 11.61	HIGL
ATOM	1744 CZ	TYR	214	21.735	60.899 123.035	1.00 11.76	HIGL HIGL
MOTA	1745 OH	TYR	214	20.722	59.997 123.259	1.00 12.70 1.00 14.26	HIGL
ATOM	1746 C	TYR	214 214	25.541 26.346	66.035 121.660 66.141 120.742	1.00 14.20	HIGL
MOTA MOTA	1747 O 1748 N	TYR PRO	214	25.619	66.794 122.755	1.00 14.63	HIGL
ATOM	1749 N	PRO	215	24.581	67.036 123.775	1.00 14.17	HIGL
ATOM	1750 CA	PRO	215	26.682	67.790 122.847	1.00 14.95	HIGL
MOTA	1751 CB	PRO	215	25.990	68.930 123.572	1.00 14.94	HIGL
MOTA	1752 CG	PRO	215	25.175		1.00 14.41	HIGL HIGL
ATOM	1753 C	PRO	215	27.924		1.00 15.93 1.00 16.94	HIGL
ATOM	1754 O	PRO	215	28.999	67.898 123.437	1.00 10.34	

Fig. 2 cont.

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ATOM	1755 N	PHE	216	27.778		1.00.16.00	HIGL
ATOM	1756 CA	PHE	216	28.878		1.00 16.24	HIGL
ATOM	1757 CB	PHE	216	28.350		1.00 16.24	HIGL HIGL
MOTA	1758 CG	PHE	216	27.018		1.00 16.08 1.00 15.04	HIGL
MOTA	1759 CD1	PHE	216	26.861		1.00 15.04	HIGL
MOTA	1760 CD2	PHE	216	25.924	03.31. 22	1.00 15.16	HIGL
ATOM	1761 CE1	PHE	216	25.638	64.686 127.386	1.00 14.85	HIGL
MOTA	1762 CE2	PHE	216	24.703 24.560	63.453 126.759	1.00 14.72	HIGL
ATOM	1763 CZ	PHE	216 216	29.709	64.595 124.763	1.00 16.64	$\mathtt{HIGL}$
ATOM	1764 C 1765 O	PHE	216	30.291		1.00 16.43	HIGL
ATOM ATOM	1765 N	TYR	217	29.789	64.377 123.459	1.00 17.14	HIGL
MOTA	1767 CA	TYR	217	30.582		1.00 17.62	. HIGL
ATOM	1768 CB	TYR	217	29.675		1.00 16.27	HIGL
ATOM	1769 CG	TYR	217	28.847	•=	1.00 16.34	HIGL
ATOM	1770 CD1	TYR	.217	29.440		1.00 16.29	HIGL HIGL
MOTA	1771 CE1	TYR	217	28.687		1.00 15.97 1.00 15.38	HIGL
MOTA	1772 CD2	TYR	217	27.477	61.232 123.131 60.477 124.016	1.00 13.30	HIGL
ATOM	1773 CE2	TYR	217	26.717 27.324	59.875 125.102	1.00 16.23	HIGL
ATOM	1774 CZ '	TYR	217	26.566	59.120 125.977	1.00 17.30	HIGL
MOTA	1775 OH	TYR TYR	217 217	31.605	63.723 121.909	1.00 18.43	HIGL
ATOM ATOM	1776 C 1 <b>77</b> 7 O	TYR	217	32.308	62.908 121.317	1.00 19.53	HIGL
ATOM	1777 N	SER	218	31.693	65.034 121.703	1.00 18.33	HIGL
ATOM	1779 CA	SER	218	32.616	65.598 120.724	1.00 17.79	HIGL
MOTA	1780 CB	SER	218	32.501	64.839 119.403	1.00 17.69	HIGL
ATOM	1781 OG	SER	218	33,128	65.542 118.347	1.00 18.59	HIGL HIGL
ATOM	1782 C .	SER	218	32.298	67.070 120.485	1.00 17.69 1.00 18.71	HIGL
ATOM	1783 O	SER	218	31.141	67.438 120.306	1.00 17.22	HIGL
ATOM	1784 N	ALA	219	33.321 33.104	67.912 120.476 69.337 120.252	1.00 17.23	HIGL
MOTA	1785 CA	ALA	219 219	34.382	70.118 120.554	1.00 16.44	HIGL
ATOM	·1786 CB 1787 C	ALA ALA	219	32.661	69.589 118.816	1.00 16.60	HIGL
MOTA MOTA	1788 0	ALA	219	32.258	70.696 118.467	1.00 17.34	$\mathtt{HIGL}$
ATOM	1789 N	SER	220	32.730	68.550 117.991	1.00 16.51	HIGL
ATOM	1790 CA	SER	220	32.355	68.641 116.581	1.00 16.08	HIGL
ATOM	1791 CB	SER	220	32.954	67.466 115.809	1.00 15.86	HIGL
ATOM	1792 OG	SER	220	34.364	67.460 115.917	1.00 16.86 1.00 15.46	HIGL HIGL
MOTA	1793 C	SER	220	30.857	68.682 116.317 69.049 115.229	1.00 13.40	HIGL
MOTA	1794 O	SER	220	30.432 30.061	68.300 117.309	1.00 15.99	HIGL
ATOM	1795 N	ALA	221 221	28.606	68.279 117.164	1.00 16.78	HIGL
ATOM	1796 CA 1797 CB	ALA ALA	221	27.995	67.427 118.271	1.00 16.23	HIGL
MOTA MOTA	1797 CB	ALA	221	27.969	69.673 117.164	1.00 17.33	HIGL
ATOM	1799 0	ALA	221	27.074	69.959 117.963	1.00 17.73	HIGL
ATOM	1800 N	THR	222 -	28.422	70.534 116.260	1.00 17.34	HIGL
MOTA	1801 CA	THR	222	27.889	71.888 116.168	1.00 17.44	HIGL HIGL
MOTA	1802 CB	THR	222	28.805	72.788 115.326	1.00 16.76 1.00 16.54	HIGL
MOTA	1803 OG1		222	28.859	72.290 113.988 72.801 115.899	1.00 15.34	HIGL
MOTA	1804 CG2	THR	222	30.211	71.891 115.531	1.00 17.40	HIGL
MOTA	1805 C	THR	222	26.505 26.189	71.044 114.692	1.00 19.58	HIGL
MOTA	1806 O	THR LEU	222 223	25.675	72.842 115.933	1.00 18.21	HIGL
MOTA MOTA	1807 N 1808 CA	LEU	223	24.338	72.949 115.374	1.00 18.34	HIGL
MOTA	1809 CB	LEU	223	23.611	74.143 115.991	1.00 18.27	HIGL
MOTA	1810 CG	LEU	223	23.370	74.045 117.500	1.00 19.89	HIGL
MOTA	1811 CD1		223	22.888		1.00 19.53	HIGL
ATOM	1812 CD2	LEU	223	22.340	72.943 117.786	1.00 19.06	HIGL HIGL
MOTA	1813 C	LEU	223	24.437	73.122 113.860	1.00 18.82	HIGL
MOTA	1814 0	LEU	223	23.605		1.00 20.15 1.00 18.59	HIGL
ATOM	1815 N	ASP	224	25.457		1.00 18.39	HIGL
MOTA	1816 CA	ASP	224	25.669 26.858		1.00 18.84	HIGL
ATOM	1817 CB 1818 CG	ASP ASP	224 224	26.468		1.00 18.91	HIGL
MOTA MOTA	1819 CG		224	25.286		1.00 19.14	HIGL

Fig. 2 cont.

			•				
			•	74	4/174		
ATOM	1820 OD2	ASP	224	27.355		1.00 19.90 1.00 19.58	HIGL
MOTA	1821 C	ASP	224	25.915	72.793 111.214	1.00 19.38	HIGL HIGL
MOTA	1822 0	ASP	224	25.341	72.583 110.146 71.939 111.750	1.00 20.23	HIGL
ATOM	1823 N	SER	225	26.785 27.095	70.664 111.112	1.00 19.06	HIGL
ATOM	1824 CA	SER	225 225	28.155	69.908 111.907	1.00 18.84	HIGL
MOTA	1825 CB	SER SER	225	29.403	70.567 111.840	1.00 18.91	HIGL
ATOM ATOM	1826 OG 1827 C	SER	225	25.838	69.811 110.997	1.00 19.40	HIGL
ATOM	1828 0	SER	225	25.601	69.186 109.968	1.00 19.64	HIGL
ATOM	1829 N	LEU	226	25.039	69.774 112.058	1.00 19.24	HIGL
MOTA	1830 CA	LEU	226	23.799	69.009 112.026	1.00 19.90	HIGL
MOTA	1831 CB	TEU	226	23.069	69.103 113.372	1.00 18.41	HIGL
MOTA	1832 CG	LEU	226	21.655	68.517 113.419	1.00 18.06 1.00 17.29	HIGL HIGL
MOTA	1833 CD1	LEU	226	21.698	67.027 113.124 68.768 114.786	1.00 17.25	HIGL
MOTA	1834 CD2	LEU	226	21.042	69.628 110.925	1.00 20.05	HIGL
MOTA	1835 C	LEU	226 226	22.369	68.932 110.086	1.00 19.89	HIGL
ATOM ATOM	. 1836 O · 1837 N	LEU · ARG	227	22.883	70.951 110.941	1.00 20.56	HIGL
MOTA	1836 CA	ARG	227	22.127	71.717 109.965	1.00 22.15	HIGL
ATOM	1839 CB	ARG	227.	22.374	73.203 110.200	1.00 23.23	${\tt HIGL}$
ATOM	.1840 CG	ARG	227	21.847	74.113 109.125	1.00 23.67	HIGL
MOTA	1841 CD	ARG	227	20.585	74.801 109.561	1.00 25.35	HIGL
MOTA	1842 NE	ARG	227	20.264	75.881 108.636	1.00 27.51 1.00 27.97	${\tt HIGL}$
MOTA	1843 CZ	ARG	227	20.963	77.007 108.534 77.213 109.308	1.00 27.97	HIGL
MOTA	1844 NH1 1845 NH2	ARG	227 227	22.025 20.609	77.919 107.639	1.00 28.04	HIGL
MOTA MOTA	1846 C	ARG ARG	227	22.532	71.349 108.541	1.00 22.77	HIGL
ATOM	1847 0	ARG	227	21.682	71.091 107.685	1.00 23.17	HIGL
ATOM	1848 N	ARG	<b>22</b> B .	23.835	71.337 108.292	1.00 22.62	HIGL
ATOM	1849 CA	ARG	228	24.351	71.005 106.974	1.00 23.23	HIGL
ATOM	1850 CB	ARG	228	25.854	71.275 106.907	1.00 25.19 1.00 27.85	HIGL HIGL
MOTA	1851 CG	ARG	228	26.497 27.951	70.809 105.611 71.218 105.576	1.00 27.83	HIGL
ATOM ATOM	1852 CD 1853 NE	ARG ARG	228 228	28.217	72.426 104.784	1.00 34.16	HIGL
MOTA	1854 CZ	ARG	228	27.482	73.539 104.787	1.00 34.92	HIGL
ATOM	1855 NH1	ARG	228	26.385	73.644 105.537	1.00 34.00	HIGL
ATOM	1856 NH2	ARG	228	27.869	74.572 104.049	1.00 34.79	HIGL
MOTA	1857 C	ARG	228	24.106	69.553 106.623 69.233 105.511	1.00 21.71 1.00 21.40	HIGL HIGL
ATOM	1858 O	ARG	228 229	23.697 24.372	68.677 107.583	1.00 20.74	HIGL
MOTA MOTA	1859 N 1860 CA	SER	229	24.209	67.248 107.385	1.00 19.19	HIGL
ATOM	1861 CB	SER	229	24.596	66.499 108.657	1.00 17.46	HIGL
ATOM	1862 OG	SER	229	24.667	65.112 108.415	1.00 16.03	HIGL
ATOM	1863 C	SER	229	22.778	66.920 106.985	1.00 19.19	HIGL
MOTA	1864 O	SER	229	22.551	66.215 106.001	1.00 19.76 1.00 18.51	HIGL HIGL
ATOM	1865 N	LEU	230	21.816	67.443 107.738 67.200 107.437	1.00 18.83	HIGL
MOTA MOTA	1866 CA 1867 CB	LEU	230 230	20.414 19.513	67.904 108.459	1.00 18.57	HIGL
ATOM	1868 CG	LEU	230	19.748	67,471 109.906	1.00 18.99	HIGL
ATOM	1869 CD1	LEU	230	18.765	68.159 110.830	1.00 18.90	. HIGL
MOTA	1870 CD2	LEU	230	19.611	65.966 110.011	1.00 19.09	HIGL
MOTA	1871 C	LEU	230	20.072	67,673 106.025	1.00 18.43	HIGL HIGL
MOTA	1872 0	LEU	230	19.440	66.944 105.261 68.887 105.678	1.00 18.80 1.00 17.99	HIGL
MOTA	1873 N 1874 CA	ASN ASN	231 _. 231	20.492 20.222		1.00 17.50	HIGL
MOTA MOTA	1875 CB	ASN	231	20.775		1.00 20.27	HIGL
MOTA	1876 CG	ASN	231	19.831	71.884 104.755	1.00 21.88	HIGL
ATOM	1877 OD1		231	18.703	72.029 104.276	1.00 23.81	HIGL
ATOM	1878 ND2		231	20.284		1.00 21.50	HIGL
MOTA	1879 C	ASN	231	20.815		1.00 18.28	HIGL HIGL
MOTA	1880 O	ASN	231	20.164		1.00 17.76	HIGL
ATOM	1881 N 1882 CA	ASN ASN	232 232	22.042 22.703		1.00 17.00	HIGL
MOTA MOTA	1883 CB	ASN	232	24.141		1.00 17.29	HIGL
ATOM	1884 CG	ASN	232	25.037		1.00 16.38	HIGL

25:.037 68:116 102:915 Fig. 2 cont.

# 75/174 69.141 102.334 1.00 15.50 HIGL 232 24.686 1885 OD1. ASN MOTA 1.00 16.64 HIGL 68.005 103.521 232 26.213 ATOM 1886 ND2 ASN 65.872 102.375 1.00 18.25 HIGL 21.948 21.748 232 ASN MOTA 1887 C 1.00 17.98 65.387 101.259 HIGL 232 1888 O ASN ATOM 1.00 18.52 65.298 103.501 HIGL 21.536 233 MET MOTA 1889 N 1.00 18.43 HIGL 20.805 64.033 103.507 233 . ATOM 1890 CA MET 20.538 -63.589 104.951 21.795 63.269 105.754 1.00 18.18 HIGL 233 ATOM 1891 CB MET HIGL 1.00 18.25 233 MET ATOM 1892 CG 63.063 107.531 1.00 19.43 HIGL 233 233 21.474 MET MOTA 1893 SD 61.766 107.504 1.00 17.54 HIGL 20.199 MOTA 1894 CE MET 64.177 102.758 1.00 18.12 HIGL 233 233 19.485 MET ATOM 1895 C 1.00 18.23 HIGL 63.394 101.851 19.183 1896 O MET MOTA 1.00 17.24 1.00 16.91 65.186 103.146 HIGL 234 234 18.707 VAL 1897 N ATOM 65.455 102.530 HIGL 17.411 1898 CA VAL ATOM 1.00 15.88 1.00 15.35 16.744 + 66.687 103.179 15.486 67.056 102.420 16.413 66.390 104.638 HIGL 234 234 VAL 1899 CB MOTA HIGL 1900 CG1 ATOM . VAL HIGL 1.00 15.47 234 VAL 1901 CG2 ATOM 1.00 16.63 HIGL 17.502 65.678 101.017 234 ATOM 1902 C VAL 1.00 16.27 1.00 16.80 HIGL 234 235 65.045 100.245 16.784 VAL 1903 O MOTA 66.575 100.603 HIGL 18.391 MOTA 1904 N SER 1.00 17.13 1.00 17.78 1.00 17.56 1.00 16.92 HIGL 235 235 66.882 99.190 SER 18.573 MOTA 1905 CA HIGL 19.578 68,023 99.024 1906 CB SER ATOM 235 235 235 236 HIGL 97.656 19.784 68.317 1907 OG SER ATOM HIGL 65.677 65.562 19.049 98.384 SER 1908 C ATOM 1.00 17.15 HIGL 97.190 18.768 MOTA 1909 O SER HIGL 99.045 1.00 16.40 19.759 64.774 ATOM 1910 N ARG 1.00 16.55 1.00 17.11 HIGL 63.595 98.384 1911 CA 236 20.290 ARG ATOM HIGL 236 21.568 63.161 99.084 ARG MOTA . 1912 CB 1.00 18.73 1.00 19.62 1.00 24.11 1.00 25.92 98.562 HIGL 236 236 61.872 22.156 ATOM 1913 CG ARG HIGL 22.995 62.074 97.321 MOTA 1914 CD ARG 23.973 23.732 22.532 97.231 HIGL 60.997 1915 NE 236 ARG MOTA HIGL 59.794 59.505 96.710 236 ARG ATOM 1916 CZ 236 236 96.205 1.00 24.62 HIGL ARG MOTA 1917 NH1 1.00 25.67 HIGL 24.691 19.343 58.867 96.725 ARG MOTA 1918 NH2 1.00 16.75 1.00 15.62 HIGL 62.400 98.298 ARG 236 ATOM 1919 C 19.259 18.637 HIGL 97.259 236 61.740 ARG MOTA 1920 O HIGL 1.00 16.82 62.111 99.385 TRP 237 1921 N ATOM 17.745 18.224 1.00 16.41 HIGL 237 60.961 99.390 MOTA 1922 CA TRP 59.966 100.453 1.00 16.05 HIGL 237 1923 CB TRP MOTA 100.040 1.00 14.89 HIGL TRP 237 19.505 59.294 1924 CG ATOM 1.00 14.04 1.00 14.30 HIGL 20.817 59.526 100.571 ATOM 1925 CD2 TRP 237 HIGL 21.717 21.322 237 58.738 99.817 1926 CE2 TRP MOTA 1.00 13.86 1.00 15.03 HIGL 60.327 101.604 1927 CE3 TRP 237 MOTA HIGL 19.659 20.983 99.023 58.398 237 · TRP ATOM 1928 CD1 1.00 14.90 1.00 13.70 98.882 HIGL 58.060 1929 NE1 TRP 237 ATOM HIGL 58.727 100.061 237 23.097 TRP 1930 CZ2 MOTA 22.695 23.566 60.319 101.847 HIGL 1.00 13.61 MOTA 1931 CZ3 TRP 237 HIGL 237 237 1.00 14.26 59.522 101.074 TRP 1932 CH2 MOTA 16.266 1.00 16.86 HIGL 99.557 61.281 MOTA 1933 C TRP HIGL 1.00 18.12 15.430 15.953 60.383 99.522 237 TRP 1934 O ATOM 99.732 1.00 16.74 HIGL 62.562 238 MOTA 1935 N GLY 1.00 16.56 HIGL 14.574 13.714 GLY 238 .62.995 99.869 1936 CA MOTA 1.00 17.47 1.00 17.51 62.388 100.966 HIGL 1937 C 1938 O MOTA GLY 238 HIGL 12.486 14.330 62.346 100.836 GLY 238 MOTA 61.933 102.053 1.00 16.96 HIGL 239 1939 N LYS MOTA HIGL 1.00 16.74 61.339 103.146 1940 CA LYS 239 13.564 MOTA HIGL 14.327 60.152 103.724 1.00 16.66 239 1941 CB LYS MOTA 1.00 17.05 HIGL 59.053 102.730 239 14.606 1942 CG LYS MOTA 58.511 102.175 HIGL 13.312 1.00 15.57 1943 CD LYS 239 ATOM 57.342 101.262 1.00 14.83 HIGL LYS 239 13.561 1944 CE MOTA 56.925 100.661 HIGL 12.275 1.00 14.06 239 1945 NZ LYS MOTA 1.00 16.96 HIGL 62.344 104.261 13.302 1946 C LYS 239 MOTA HIGL 1.00 17.61 63.323 104.398 14.036 1947 O LYS 239 MOTA 1.00 17.26 HIGL 240 240 12.257 62.118 105.056 GLU 1948 N MOTA 1.00 16.82 HIGL 11.985 63.016 106.181 1949 CA GLU MOTA

Fig. 2 cont.

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ATOM	1950 CB	GLU	240	10.615	62.743 106.808	1.00 17.65	HIGL HIGL
MOTA	1951 CG	GLU	240	9.430 8.116	63.085 105.923 63.080 106.690	1.00 18.86 1.00 20.65	HIGL
MOTA MOTA	1952 CD 1953 OE1	GLU GLU	240 240	7.818	62.067 107.353	1.00 21.31	HIGL
ATOM	1954 OE2	GLU	240	7.381	64.091 106.634	1.00 21.43	HIGL
ATOM	1955 C	GLU	240	13.088	62.751 107.209	1.00 16.31 1.00 15.76	HIGL HIGL
MOTA	1956 0	GLU	240 241	13.562 13.493	61.621 107.360 63.793 107.917	1.00 15.70	HIGL
MOTA MOTA	1957 N 1958 CA	VAL VAL	241	14.571	63.666 108.883	1.00 15.54	HIGL
MOTA	1959 CB	VAL	241	15.754	64.547 108.432	1.00 14.72	HIGL
MOTA	1960 CG1	VAL	241	16.789	64.623 109.501 63.974 107.178	1.00 17.13 1.00 15.36	HIGL HIGL
MOTA	1961 CG2 1962 C	VAL VAL	241 241	16.361 14.149	64.045 110.299	1.00 15.60	HIGL
ATOM ATOM	1963 0	VAL	241	13.161	64.758 110.495	1.00 16.76	HIGL
MOTA	1964 N	ALA	242	14.900	63.573 111.290	1.00 14.40	HIGL HIGL
MOTA	1965 · CA	ALA	242	14.577 13.286	63.888 112.673 63.177 113.082	1.00 13.72 1.00 12.95	HIGL
MOTA MOTA	1966 CB 1967 C	ALA ALA	242 242	15.681	63.519 113.645	1.00 13.47	HIGL
ATOM	1968 0	ALA	242	16.428	62.561 113.429	1.00 13.51	HIGL
MOTA	1969 N	VAL	243	15.791	64.303 114.711	1.00 13.04 1.00 13.08	HIGL HIGL
MOTA	1970 CA	VAL	243 243	16.760 17.192	64.023 115.758 65.294 116.497	1.00 13.08	HIGL
MOTA MOTA	1971 CB 1972 CG1	VAL VAL	243	17.132	64.924 117.771	1.00 12.23	HIGL
ATOM	1973 CG2	VAL	243	18.088	66.125 115.604	1.00 12.08	HIGL
MOTA	1974 C	VAL	243	15.964	63.139 116.701 63.593 117.346	1.00 13.56 1.00 13.37	. HIGL HIGL
ATOM	1975 O 1976 N	VAL VAL	243 244	15.014 16.328	61.866 116.754	1.00 14.00	HIGL
MOTA MOTA	1977 CA	VAL	244	15.608	60.927 117.593	1.00 14.42	HIGL
MOTA	1978 CB	VAL	244	15.476	59.569 116.877	1.00 13.73	HIGL
ATOM	1979 CG1	VAL	244	14.782 16.831	59.774 115.548 58.955 116.653	1.00 13.75 1.00 12.09	HIGL HIGL
ATOM ATOM	1980 CG2 1981 C	VAL VAL	244 244	16.242	60.742 118.965	1.00 15.18	HIGL
ATOM	1982 0	VAL	244	15.748	59.965 119.783	1.00 14.93	HIGL
MOTA	1983 N	<b>GT</b> U	245	17.320	61.479 119.218	1.00 15.57 1.00 16.66	HIGL HIGL
MOTA	1984 CA	GLU	245	18.023 18.933	61.397 120.490 60.176 120.517	1.00 15.00	HIGL
ATOM ATOM	1985 CB 1986 CG	GLU	245 · 245	18,295	58.883 120.921	1.00 19.86	HIGL
ATOM	1987 CD	GLU	245	19.325	57.778 121.021	1.00 21.19	HIGL
ATOM	1988 OE1	GLU	245	20.395	58.018 121.624 56.673 120.502	1.00 22.19 · 1.00 22.22	HIGL HIGL
ATOM ATOM	1989 OE2 1990 C	GLU	245 245	19.071 18.892	62.616 120.780	1.00 17.25	HIGL
ATOM	1991 0	GLU	245	19.756	62.984 119.979	1.00 17.63	HIGL
MOTA	1992 N	THR	246	18.675	63.226 121.938	1.00 16.70	HIGL HIGL
ATOM	1993 CA	THR	246	19.468 19.133	64.372 122.350 65.632 121.534	1.00 16.24 1.00 16.24	HIGL
MOTA MOTA	1994 CB 1995 OG1	THR THR	246 246	20.097	66.649 121.831	1.00 16.02	$\mathtt{HIGL}$
ATOM	1996 CG2	THR	246	17.737	66.146 121.872	1.00 14.97	HIGL
ATOM	1997 C	THR	246	19.221	64.650 123.824	1.00 16.42 1.00 16.91	HIGL HIGL
MOTA	1998 O	THR	246 247	18.165 20.206	64.315 124.356 65.256 124.475	1.00 16.16	HIGL
ATOM ATOM	1999 N 2000 CA	ASN ASN	247	20.125	65.586 125.891	1.00 16.42	HIGL
ATOM	2001 CB	ASN	247	20.753	64.482 126.754	1.00 18.32	HIGL
MOTA	2002 CG	ASN	247	19.876	63.247 126.900 62.190 127.311	1.00 19.99 1.00 20.70	HIGL HIGL
ATOM ATOM	2003 OD1 2004 ND2		247 247	20.357 18.593	63.374 126.587	1.00 19.85	HIGL
ATOM	2004 ND2	ASN	247	20.931	66.850 126.139	1.00 16.21	HIGL
ATOM	2006 O	ASN	247	21.769	67.235 125.329	1.00 16.56	HIGL HIGL
ATOM	2007 N	TRP	248	20.664	67.491 127.267 68.666 127.680	1.00 15.12 1.00 14.40	HIGL
ATOM	2008 CA 2009 CB	TRP TRP	248 248	21.407 20.750	69.965 127.235	1.00 14.45	HIGL
ATOM ATOM	2010 CB	TRP	248	21.582	71.144 127.642	1.00 13.41	HIGL
ATOM	2011 CD2	TRP	248	22.789	71.592 127.020	1.00 12.55	HIGL
MOTA	2012 CE2		248	23.279		1.00 13.08 1.00 12.85	HIGL HIGL
MOTA MOTA	2013 CE3 2014 CD1		248 248	23.508 21.391	71.183 123.890	1.00 13.60	HIGL
W TOTA	2014 CDI		270				

Fig. 2 cont.

# 77/174 72.870 128.824 1.00 12.73 HIGL 22,408 248 MOTA 2015 NE1 TRP 73.352 127.458 1.00 12.54 HIGL 24.457 248 ATOM 2016 CZ2 TRP HIGL 71.857 125.564 1.00 11.70 24.679 TRP 248 ATOM 2017 CZ3 HIGL 1.00 12.92 25.141 72.929 126.347 248 ATOM 2018 CH2 TRP HIGL 68.570 129.188 1.00 14.62 2019 C, 21.404 24B MOTA TRP 1.00 15.22 HIGL ~ 20.351 68.434 129.802 248 MOTA 2020 O TRP HIGL . 22.585 68.633 129.808 1.00 14.33 249 MOTA 2021 N PRO HIGL 1.00 14.04 68.623 129.197 23.925 249 2022 CD MOTA PRO .68.532 131.260 1.00 14.94 HIGL 22.673 2023 CA 249 PRO ATOM 1.00 14.74 HIGL 24.099 68.041 131.468 249 2024 CB PRO MOTA 1.00 13.70 HIGL 24.836 68.752 130.390 MOTA 2025 CG PRO 249 HIGL 249 249 1.00 15.82 22.381 69.783 132.066 2026 C PRO MOTA 22.594 HIGL 1.00 16.63 70.895 131.604 MOTA 2027 O PRO 1.00 17.24 HIGL 21.882 69.578 133.282 250 2028 N THR ATOM 21.603 70.672 134.207 1.00 17.83 HIGL MOTA 2029 CA THR 250 20.308 1.00 16.40 HIGL 250 70.451 134.975 2030 CB ŢHR MOTA 20.478 1.00 16.53 HIGL 69.353 135.875 ATOM 2031 OG1 THR 250 . 1.00 17.51 HIGL 250 · 19.174 70.153 134.014 2032 CG2 THR ATOM 22.758 1.00 18.49 HIGL 70.645 135.206 250 THR ATOM 2033 C HIGL .,1.00 19.82 250 22.875 71.509 136.078 2034 0 THR MOTA . HIGL 23,601 69.627 135.057 1.00 18.20 251 MOTA 2035 N SER 1.00 17.27 HIGL 251 24.769 69.426 135.897 2036 CA SER MOTA 1.00 16.80 HIGL 24.373 68.700 137.181 SER 251 ATOM 2037 CB 1.00 16.67 HIGL 25.486 25.769 68.537 138.046 251 251 2038 OG SER ATOM 1.00 17.65 68.579 135.122 HIGL 2039 C SER MOTA 1.00 17.82 HIGL 67.476 134.682 25.444 251 ATOM 2040 O SER 252 ... HIGL 1.00 17.77 69.099 134.936 26.975 MOTA 2041 N CYS 252 252 1.00 19.00 HIGL 68.359 134.218 28.012 CYS ATOM 2042 CA 68.791 134.751 69.460 134.069 HIGL 1.00 18.46 29.375 2043 C CYS ATOM 1.00 18.37 HIGL 252 252 30.142 CYS MOTA 2044 O HIGL 6B.611 132.703 1.00 19.48 27.940 2045 CB CYS MOTA 1.00 21.91 1.00 18.43 HIGL 67.349 131.755 2046 SG CYS 252 28.860 MOTA 68.402 135.992 67.630 136.898 HIGL 253 · 29.687 ATOM 2047 N PRO 1.00 17.81 HIGL 253 253 28.822 2048 CD PRO ATOM 1.00 18.32 1.00 17.88 1.00 18.40 1.00 18.83 HIGL 68.739 136.650 30.950 MOTA 2049 CA PRO HIGL 68.130 138.038 PRO 253 30.789 2050 CB ATOM HIGL 68.078 138.228 68.204 135.952 253 29.313 PRO ATOM 2051 CG HIGL 253 253 PRO 32.191 2052 C ATOM HIGL 33.213 68.887 135.900 MOTA 2053 O PRO 1.00 19.26 1.00 19.93 66.989 135.414 66.378 134.766 HIGL 32.102 TYR 254 2054 N ATOM HIGL 33.256 33.782 254 TYR MOTA 2055 CA 1.00 19.85 HIGL 65.223 135.616 TYR 254 2056 CB MOTA 1.00 19.85 HIGL 33,909 65.574 137.076 254 TYR MOTA 2057 CG 1.00 18.49 1.00 18.20 HIGL 65.468 137.934 2058 CD1 TYR 254 32.816 ATOM HIGL 32.915 65.836 139.268 254 ATOM 2059 CE1 TYR 66.060 137.594 1.00 19.80 HIGL 254 35.112 MOTA 2060 CD2 TYR 1.00 18.50 HIGL 254 254 35.218 34.115 66.434 138.930 66.319 139.755 TYR MOTA 2061 CE2 1.00 18.08 1.00 18.79 HIGL ATOM 2062 CZ TYR HIGL 254 34.207 66.697 141.065 TYR 2063 OH MOTA HIGL 65.873 133.357 1.00 21.05 33.031 MOTA 2064 C TYR 254 1.00 22.11 HIGL 254 32.995 64.667 133.128 TYR MOTA 2065 O 1.00 21.11 1.00 20.35 32.898 66.789 132.387 HIGL 255 PRO MOTA 2066 N HIGL 33.042 32.684 PRO 255 68.251 132.488 2067 CD MOTA HIGL 66.391 130.999 1.00 21.28 2068 CA PRO 255 ATOM 32.472 33.369 1.00 21.29 HIGL 67.724 130.299 2069 CB 255 PRO MOTA 68.632 131.075 2070 CG 2071 C 1.00 20.00 HIGL PRO 255 MOTA 1.00 22.18 HIGL 33.910 65.667 130.469 PRO 255 MOTA HIGL 35.034 33.698 1.00 22.28 66.059 130.767 2072 O PRO 255 ATOM 1.00 23.41 HIGL 256 64.613 129.686 2073 N ARG ATOM 1.00 24.09 1.00 25.18 63.872 129.118 HIGL 34.817 256 2074 CA ARG ATOM HIGL 62.462 128.702 34.386 256 2075 CB ARG ATOM 1.00 28.36 35.537 HIGL 61.602 128.198 256 MOTA 2076 CG ARG 1.00 31.88 HIGL 60.254 127.676 2077 CD 256 35.062 MOTA ARG 1.00 35.40 HIGL 36.176 59.403 127.254 ARG 256 2078 NE ATOM 1.00 36.69 HIGL 36.043 58.226 126.636 256 ATOM 2079 CZ ARG

Fig. 2 cont.

				78	3/174		
MOTA	2080 NH1	ARG	256	34.837	57.744 126.353	1.00 36.99 1.00 37.44	HIGL HIGL
ATOM	2081 NH2	ARG	256	37.122 35.354	J/, JEG ===:===	1.00 37.44	HIGL
MOTA MOTA	2082 C 2083 O	ARG ARG	256 256	36.538	64.553 127.593	1.00 23.73	HIGL
ATOM	2083 O	TYR	257	34.481	65.357 127.226	1.00 22.94	HIGL
MOTA	2085 CA	TYR	257	34.893	66.107 126.054	1.00 23.27 1.00 23.86	HIGL HIGL
ATOM	2086 CB	TYR TYR	257 257	34.287 34.485	65.502 124.788 64.018 124.653	1.00 23.00	HIGL
ATOM ATOM	2087 CG 2088 CD1	TYR	257	33.570	63.124 125.204	1.00 25.20	HIGL
ATOM	2089 CE1	TYR	257	33.742	61.747 125.077	1.00 26.62	HIGL HIGL
MOTA	2090 CD2	TYR	257	35.585	63.502 123.970 62.128 123.838	1.00 24.88 1.00 26.37	HIGL
ATOM ATOM	2091 CE2 2092 CZ	TYR TYR	257 257	35.771 34.843	61.255 124.395	1.00 27.15	HIGL
ATOM	2092 OE	TYR	257	35.018	59.895 124.276	1.00 27.95	HIGL
ATOM	2094 C	TYR	257	34.480	67.567 126.127	1.00 23.40 1.00 23.44	HIGL HIGL
ATOM	2095 O	TYR	257 258	33.530 35.204	67.929.126.813 68.406 125.404	1.00 23.44	HIGL
MOTA MOTA	2096 N 2097 CA	GLN GLN	258	34.886	69.816 125.367	1.00 23.32	HIGL
ATOM	2098 CB	GLN	258	35.998	70.566. 124.641	1.00 25.30	HIGL . HIGL
MOTA	2099 CG	GLN	258	35.814	72.063 124.549 72.781 124.380	1.00 29.69 1.00 33.22	HIGL
ATOM	2100 CD 2101 OE1	GLN GLN	258 258	37.146 37.199	73.936 123.943	1.00 34.85	HIGL
ATOM ATOM	2102 NE2	GLN	258	38.234	72.099 124.741	1.00 33.71	HIGL
ATOM	2103 C	GLN	258	33.573	69.922 124.608	1.00 21.85	HIGL HIGL
MOTA	2104 0	GLN	258	33.359 . 32.680	69.209 123.632 70.784 125.067	1.00 21.62 1.00 20.74	HIGL
ATOM ATOM	2105 N 2106 CA	PHE PHE	259 259	31.405	70.954 124.390	1.00 20.36	HIGL
ATOM	2107 CB	PHE	259	30.415	71.652 125.318	1.00 20.17	HIGL
MOTA	2108 CG	PHE	259	29.691	70.718 126.243 69.756 126.969	1.00 20.50 1.00 20.48	HIGL HIGL
MOTA	2109 CD1 2110 CD2	PHE PHE	259 259	30.383 · 28.310	70.803 126.391	1.00 19.48	HIGL .
MOTA MOTA	2110 CD2	PHE	259	29.707	68.887 127.830	1.00 21.21	HIGL
ATOM	2112 · CE2	PHE	259	27.629	69.943 127.246	1.00 19.74 1.00 20.03	$\mathtt{HIGL}$
MOTA	2113 CZ	PHE	259 259	28.328 31.578	68.982 127.968 71.769 123.110	1.00 20.03	HIGL
ATOM ATOM	2114 C 2115 O	PHE PHE	259	32.557	72.486 122.953	1.00 19.93	HIGL
ATOM	2116 N	PRO	260	30.637	71.651 122.165	1.00 20.85	HIGL HIGL
MOTA	2117 CD	PRO	260	29.527	70.687 122.073 72.427 120.924	1.00 20.21 1.00 21.17	HIGL
ATOM ATOM	2118 CA 2119 CB	PRO PRO	260 260	30.766 29.506	72.048 120.156	1.00 21.01	HIGL
MOTA	2120 CG	PRO	260	29.291	70.617 120.584	1.00 20.56	HIGL
ATOM	2121 C	PRO	260	30.837	73.928 121.239	1.00 21.74 1.00 21.19	HIGL HIGL
ATOM	2122 0	PRO	260 261	30.163 31.657	74.414 122.150 74.654 120.487	1.00 21.19	HIGL
MOTA MOTA	2123 N 2124 CA	ALA ALA	261	31.830	76.089 120.697	1.00 22.38	HIGL
MOTA	2125 CB	ALA	261	32.836	76.636 119.697	1.00 21.76	HIGL HIGL
ATOM	2126 C	ALA	261	30.540 30.411	76.901 120.621 77.929 121.290	1.00 22.55 1.00 23.31	HIGL
MOTA MOTA	2127 O 2128 N	ALA ASP	261 262	29.586	76.449 119.814	1.00 22.59	HIGL
ATOM	2129 CA	ASP	262	28.331	77.173 119.674	1.00 23.66	HIGL
MOTA	2130 CB	ASP	262	27.570	76.715 118.426	1.00 24.06 1.00 25.82	HIGL HIGL
ATOM	2131 CG	ASP	262 262	27.368 27.333	75.206 118.369 74.550 119.435	1.00 25.02	HIGL
ATOM ATOM	2132 OD1 2133 OD2		262	27.224	74.677 117.243	1.00 26.76	HIGL
MOTA	2134 C	ASP	262	27.401	77.095 120.878	1.00 24.22	HIGL
ATOM	2135 0	ASP	262 263	26.449 27.661	77.866 120.965 76.174 121.802	1.00 24.88 1.00 25.01	HIGL
MOTA MOTA	2136 N 2137 CA	VAL VAL	263	26.803	76.042 122.976	1.00 26.27	HIGL
MOTA	2138 CB	VAL	263	26.062	74.68D 122.990	1.00 25.93	HIGL
MOTA	2139 CG1		263	25.179	74.554 121.757		HIGL HIGL
ATOM	2140 CG2		263 263	27.056 27.525	73.540 123.063 76.211 124.309		HIGL
MOTA MOTA	2141 C 2142 O	VAL VAL	263	26.931	76.014 125.365	1.00 27.35	HIGL
MOTA	2143 N	ARG	264	28.799	76.590 124.257	1.00 29.44	HIGL HIGL
ATOM	2144 CA	ARG	264	29.595	76.782 125.466	1.00 31.30	111011

Fig. 2 cont.

				79	0/174		
ATOM	2145 CB	ARG .	264	31.066	76.969 125.092	1.00 32.75	HIGL
ATOM	2146 CG	ARG	264	31.645	75.755 124.389	1.00 35.35 1.00 37.11	HIGL HIGL
ATOM	2147 CD	ARG	264	33.075	75.968 123.917 74.810 123.161	1.00 37.11	HIGL
	2148 NE	ARG	264 264	33.550 34.738	74.727 122.571	1.00 38.26	HIGL
ATOM ATOM	2149 CZ 2150 NH1	ARG ARG	264	35.590	75.742 122.646	1.00 38.84	HIGL
ATOM	2150 NH1 2151 NH2	ARG	264	35.072	73.629 121.903	1.00 37.21	HIGL
ATOM	2152 C	ARG	264	29.110	77.968 126.294	1.00 31.82	HIGL HIGL
ATOM	2153 0	ARG	264	29.649	78.256 127.360 78.648 125.796	1.00 32.57 1.00 31.94	HIGL
MOTA	2154 N	asn Asn	265 265	28.086 27.508	79.801 126.480	1.00 31.74	HIGL
MOTA MOTA	2155 CA 2156 CB	ASN	265	27.189	80.893 125.464	1.00 33.87	HIGL
ATOM	2157 CG	ASN	265	26.419	80.357 124.264	1.00 35.62	HIGL
ATOM	2158 OD1	ASN	265	25.213	80.600 124.115	1.00 36.81 1.00 35.24	HIGL HIGL
ATOM	2159 ND2	ASN	265	27.113 26.227	79.608 123.407 79.376 127.175	1.00 33.24	HIGL
ATOM ATOM	2160 C 2161 O	ASN ASN	265 265	25.738	80.064 128.067	1.00 31.10	HIGL
MOTA	2162 N	VAL	266	25.685	78.240 126.746	1.00 28.31	HIGL
ATOM	2163 CA	VAL	266	24.455	77.701 127.307	1.00 25.56	HIGL
MOTA	2164 CB	VAL	266	23.844	76.635 126.374	1.00 25.88 1.00 25.25	HIGL HIGL
ATOM	2165 CG1	VAL	266	22.547 23.594	76.096 126.970 77.241 124.992	1.00 23.23	HIGL
ATOM ATOM	2166 CG2 2167 C	VAL VAL	266 266	24.755	77.087 128.668	1.00 23.91	HIĢL
ATOM	2168 0	VAL	266	25.624	76.228 128.798	1.00 23.76	HIGL
ATOM	2169 N	PRO	267	24.038	77.534 129.706	1.00 21.98	HIGL HIGL
ATOM	2170 CD	PRO	267	23.034	78.615 129.662 77.047 131.075	1.00 20.37 1.00 20.98	HIGL
MOTA	2171 CA 2172 CB	PRO PRO	267 267	24.216 23.483	78.099 131.899	1.00 20.76	HIGL
ATOM ATOM	2172 CB 2173 CG	PRÓ	267	22.349	78.475 130.996	1.00 20.01	HIGL
ATOM	2174 C	PRO	267	23.670	75.655 131.340	1.00 20.67	HIGL
ATOM	2175 O	PRO T	267	22.759	75.190 130.652	1.00 20.51 1.00 20.18	HIGL HIGL
MOTA	2176 N	PHE	268 268	24.239 23.755	74.985 132.338 73.668 132.713	1.00 20.10	HIGL
ATOM ATOM	2177 CA 2178 CB	PHE	268	24.863	72.819 133.338	1.00 19.33	HIGL
ATOM	2179 CG	PHE	268	26.001	72.540 132.405	1.00 18.57	HIGL
MOTA	2180 CD1	PHE	268	25.755	72.175 131.079	1.00 18.00 1.00 17.98	HIGL HIGL
ATOM	2181 CD2	PHE	268	27.320 26.802	72.663 132.837 71.941 130.196	1.00 17.94	HIGL
ATOM ATOM	2182 CE1 2183 CE2	PHE PHE	268 268	28.382	72.431 131.961	1.00 17.83	HIGL
ATOM	2184 CZ	PHE	268	28.121	72.070 130.635	1.00 18.17	HIGL
ATOM	2185 C	PHE	268	22.667	73.953 133.727	1.00 19.80	HIGL HIGL
ATOM	2186 O	PHE	268	22.942	74.140 134.916 74.020 133.234	1.00 19.98 1.00 18.90	HIGL
MOTA	2187 N 2188 CA	SER SER	269 269	21.434 20.281	74.020 133.234	1.00 18.82	HIGL
ATOM ATOM	2189 CB	SER	269	20.339	75.752 134.567	1.00 19.28	HIGL
ATOM	2190 OG	SER	269	20.163	76.667 133,494	1.00 20.35	HIGL
ATOM	2191 C	SER	269	19.021	74.133 133.243	1.00 18.90 1.00 19.79	HIGL HIGL
ATOM	2192 O	SER	269 270	19.080 17.880	73.972 132.022 74.169 133.917	1.00 17.92	HIGL
ATOM ATOM	2193 N 2194 CA	ALA ALA	270	16.604	74.030 133.245	1.00 17.69	HIGL
ATOM	2195 CB	ALA	270	15.478	74.256 134.230	1.00 17.34	HIGL
ATOM	2196 C	ALA	270	16.526	75.050 132.111	1.00 18.21	HIGL HIGL
MOTA	2197 0	ALA	270	16.018 17.033	74.752 131.028 76.254 132.359	1.00 19.17 1.00 17.66	HIGL
ATOM ATOM	2198 N 2199 CA	ALA ALA	271 271	17.033	77.307 131.346	1.00 16.71	HIGL
ATOM	2200 CB	ALA	271	17.545	78.605 131.926	1.00 16.21	HIGL
ATOM	2201 C	ALA	271	17.838	76.886 130.145	1.00 16.17	HIGL
ATOM	2202 O	ALA	271	17.407	77.035 129.006	1.00 15.94 1.00 16.09	HIGL HIGL
MOTA	2203 N	GLY	272 272	19.024 19.906	76.348 130.415 75.900 129.353	1.00 16.09	HIGL
MOTA MOTA	2204 CA 2205 C	GLY GLY	272	19.321	74.768 128.528	1.00 16.50	HIGL
ATOM	2206 O	GLY	272	19.527	74.700 127.316	1.00 16.42	HIGL
ATOM	2207 N	GLN	273	18.593	73.867 129.177	1.00 16.88	HIGL HIGL
ATOM	2208 CA	GLN	273	17.985		1.00 17.26 1.00 16.57	HIGL
ATOM	2209 CB	GLN	273	17.267	71.005 125.414	2.00 20.01	

Fig. 2 cont.

			•	. 80	)/174		
ATOM	2210 CG	GLN .	273	18.186	71.041 130.354	1.00 16.40	HIGL
MOTA	2211 CD	GLN	273			1.00 15.47 1.00 15.89	HIGL
MOTA	2212 OE1 2213 NE2	GLN GLN	273 273	16.479 17.877	68.758 131.101	1.00 15.09	HIGL
MOTA ATOM	2213 NE2 2214 C	GLN	273	16.986	73.323 127.452	1.00 18.10	HIGL
ATOM	2215 0	GLN	273	16.955	72.903 126.297	1.00 19.02	·HIGL HIGL
ATOM	2216 N	THR	274	16.172	74.275 127.901 74.899 127.058	1.00 18.71 1.00 19.11	HIGL
MOTA	2217 CA 2218 CB	THR THR	274 274	15.161 14.419	76.016 127.826	1.00 20.20	HIGL
ATOM ATOM	2218 CB 2219 OG1	THR	274	13.856	75.469 129.026	1.00 21.70	HIGL
ATOM	2220 CG2	THR	274	13.293	76.603 126.978	1.00 20.14 1.00 19.34	HIGL HIGL
MOTA	2221 C	THR	274 274	15.840 15.485	75.498 125.842 75.213 124.700	1.00 19.34	HIGL
ATOM ATOM	2222 O 2223 N	THR GLN	275	16.838	76.325 126.115	1.00 20.37	· HIGL
ATOM	2224 CA	GLN	275	17,613	76.999 125.087	1.00 21.17	HIGL
MOTA	2225 CB	GLN	275	18.747	77.761 125.766	1.00 22.42 1.00 25.01	HIGL HIGL
ATOM	2226 CG	GLN	275 275	19.418 20.454	78.828 124.942 79.578 125.759	1.00 28.13	HIGL
MOTA MOTA	2227 CD 2228 OE1	GLN GLN	275	20.205	79.943 126.918	1.00 28.91	HIGL
MOTA	2229 NE2	GLN	275	21.621	79.817 125.166	1.00 29.71	HIGL HIGL
MOTA	2230 C	GLN	275	18,180	75.997 124.077 76.167 122.866	1.00 21.54 1.00 21.25	HIGL
ATOM	2231 O 2232 N	GLN TYR	275 276	18.022 18.831	74.948 124.579	1.00 20.83	HIGL
MOTA MOTA	2232 N 2233 CA	TYR	276	19.431	73.941 123.712	1.00 20.67	HIGL
ATOM	2234 CB	TYR	276	20.283	72.961 124.528	1.00 19.62 1.00 18.90	HIGL HIGL
MOTA	·2235 CG	. TYR	276	20.995 22.193	71.923 123.681 72.222 123.020	1.00 18.90	HIGL
MOTA MOTA	2236 CD1 2237 CE1	TYR TYR	27.6 27.6	22.854	71.260 122.245	1.00 18.33	HIGL
MOTA	2238 CD2	TYR	276	20.471	70.641 123.540	1.00 18.85	HIGL
MOŢA	2239 CE2	TYR	27.6	21.114	69.677 122.769	1.00 18.77 1.00 19.64	HIGL HIGL
MOTA	2240 CZ -	TYR TYR	276 276	22.304 22.938	69.986 122.127 69.006 121.391	1.00 19.63	HIGL
MOTA MOTA	2241 OH 2242 C	TYR	276	18.406	73.150 122.907	1.00 20.77	HIGL
ATOM	2243 O	TYR	276	18.547	72.992 121.695	1.00 20.48	HIGL HIGL
MOTA	2244 N	ILE	277	17.386	72.639 123.584 71.857 122.912	1.00 21.04 1.00 21.46	HIGL
MOTA MOTA	2245 CA 2246 CB	ILE	277 277	16.361 15.303	71.345 123.913	1.00 21.68	HIGL
ATOM	2247 CG2	ILE	277	14.172	70.635 123.167	1.00 21.01	HIGL
MOTA	2248 CG1	ILE	277	15.965	70.393 124.912	1.00 20.42 1.00 21.50	t HIGL
MOTA	2249 CD1	ILE	277 277	15.058 15.685	69.950 126.033 72.690 121.841	1.00 21.85	HIGL
ATOM ATOM	2250 C 2251 O	ILE	277	15.334	72.185 120.780	1.00 21.88	HIGL
ATOM	2252 N	GLN	278	15.520	73.975 122.114	1.00 22.68	HIGL
MOTA	2253 CA	GLN	278	14.881 14.468	74.863 121.159 76.164 121.856	1.00 23.40 1.00 25.27	HIGL HIGL
MOTA MOTA	2254 CB 2255 CG	GLN GLN	278 278	13.664	77.127 120.993	1.00 28.71	HIGL
MOTA	2256 CD	GLN	· 278	12.524	77.786 121.759	1.00 31.37	HIGL
MOTA	2257 OE1	GLN	278	12.699	78.244 122.900	1.00 32.36 1.00 31.74	HIGL HIGL
ATOM	2258 NE2 2259 C	GLN GLN	278 278	11.347 15.789	77.845 121.132 75.145 119.963	1.00 22.37	HIGL
MOTA MOTA	2260 O	GLN	278	15.319	75.205 118.829	1.00 22.41	HIGL
MOTA	2261 N	SER	279	17.085	75.311 120.213	1.00 21.36	HIGL HIGL
ATOM	2262 CA	SER	279	18.042	75.563 119.137 75.775 119.697	1.00 20.77 1.00 20.20	HIGL
ATOM ATOM	2263 CB 2264 OG	SER SER	279 279	19.445 19.492	76.892 120.554	1.00 21.57	HIGL
ATOM	2265 C	SER	279	18.083	74.372 118.185	1.00 20.98	HIGL
ATOM	2266 O	SER	279	18.103	74.536 116.962	1.00 21.23 1.00 20.27	HIGL HIGL
MOTA	2267 N	JAV	280	18.102 18.141	73.172 118.762 71.945 117.983	1.00 20.27	HIGL
ATOM ATOM	2268 CA 2269 CB	VAL VAL	280 280	18.294	70.721 118.905	1.00 18.93	HIGL
ATOM	2270 CG1		280	18.277	69.436 118.088	1.00 18.16	HIGL
ATOM	2271 CG2		280	19.586	70.837 119.686	1.00 17.85 1.00 19.71	HIGL HIGL
ATOM	2272 C 2273 O	VAL VAL	280 280	16.865 16.895		1.00 19.74	HIGL
MOTA ATOM	2273 O 2274 N	ALA	281	15.744	72.229 117.746	1.00 19.63	HIGL

Fig. 2 cont.

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ATOM	2275 CA	ALA	281	14.467	72.176 117.044	1.00 19.86	HIGL
ATOM	2275 CR 2276 CB	ALA	281	13.324	72.570 117.982	1.00 19.49	HIGL
ATOM	2277 C	ALA	281	14.519	73.123 115.847	1.00 19.99	HIGL
ATOM	2278 0	ALA	281	14.070	72.782 114.751	1.00 19.99	HIGL HIGL
ATOM	2279 N	ASN	282	15.080	74.309 116.056	1.00 20.40	HIGL
ATOM	2280 CA	ASN	282	15.189	75.283 114.979	1.00 21.01	HIGL
ATOM	2281 CB	ASN	282	15.867	76.562 115.463	1.00 22.58 1.00 25.95	HIGL
MOTA	2282 CG	asn	282	15.081	77.253 116.555	1.00 23.93	HIGL
ATOM	.2283 OD1	ASN	282	13.850	77.335 116.489	1.00 25.99	HIGL
MOTA	2284 ND2	ASN	282	15.786	77.765 117.567 74.709 113.818	1.00 20.44	HIGL
MOTA	2285 C	ASN	282	15.976	74.709 113.810	1.00 21.36	HIGL
MOTA	2286 O	ASN	282	15.608 17.058	73.995 114.118	1.00 18.69	HIGL
MOTA	2287 N	VAL	283 283	17.868	73.396 113.064	1.00 18.11	HIGL
ATOM	2288 CA	VAL VAL	283	19.105	72.668 113.639	1.00 17.40	HIGL
MOTA	2289 CB 2290 CG1	VAL	283	19.738	71.771 112.581	1.00 15.51	HIGL
MOTA MOTA	2290 CG1 2291 CG2	VAL	283	20.117	73.692 114.128	1.00 15.34	HIGL
ATOM	2292 C	VAL	283	17.028	72.418 112.256	1.00 18.82	$\mathtt{HIGL}$
MOTA	2293 0	VAL	283	16.972	72.504 111.034	1.00 19.69	HIGL
ATOM	2294 N	VAL	284	16.365	71.497 112.942	1.00 19.82	HIGL
MOTA	2295 CA	VAL	284	15.518	70.514 112.277	1.00 20.48	HIGL
ATOM	2296 CB	VAL	284	14.874	69.570 113.304	1.00 19.52	HIGL
ATOM	2297 CG1	VAL	284	14.015	68.549 112.595	1.00 17.63	HIGL
ATOM	2298 CG2	VAL	284	15.956	68.896 114.132	1.00 18.42	HIGL HIGL
ATOM	2299 C	VAL	284	14.405	71.185 111.452	1.00 21.90 1.00 22.17	HIGL
MOTA	2300 O	VAL	284	14.205	70.863 110.279	1.00 22.17	HIGL
ATOM	2301 N	SER	285	13.685	72.117 112.068 72.620 111.380	1.00 22.13	HIGL
ATOM	2302 CA	SER	285	12.609	73.817 112.317	1.00 22.73	HIGL
MOTA	2303 CB	SER	285	11.936 11.369	73.153 113.426	1.00 26.28	HIGL
MOTA	2304 OG	SER	285 285	13.112	73.571 110.160	1.00 23.02	HIGL
ATOM	2305 C	ser ser	285	12.447	73.585 109.126	1.00 23.75	HIGL
MOTA	2306 O 2307 N	SER	28.6	14.279	74.203 110.282	1.00 23.31	HIGL
ATOM ATOM	2308 CA	SER	286	14.848	74.975 109.177	1.00 23.26	HIGL
MOTA	2309 CB	SER	286	16.231	75.524 109.545	1.00 22.79	HIGL
MOTA	2310 OG	SER	286	17.224	74.513 109.479	1.00 22.57	HIGL
ATOM	2311 C	SER	286	14.969	74.104 107.937	1.00 23.61	HIGL
ATOM	2312 0	SER	286	14.824	74.586 106.812	1.00 24.61	HIGL
ATOM	2313 N	VAL	287	15.227	72.817 108.150	1.00 22.94	HIGL HIGL
ATOM	2314 CA	VAL	287	15.371	71.876 107.051	1.00 22.39 1.00 21.12	· HIGL
MOTA	2315 CB	VAL	287	16.126	70.596 107.494	1.00 21.12	HIGL
MOTA	2316 CG1		287	16.217	69.617 106.341 70.952 107.989	1.00 19.96	HIGL
MOTA	2317 CG2		287	17.500 14.020	71.452 106.510	1.00 22.70	HIGL
ATOM	2318 C	VAL	287 287	13.129	71.075 107.266		HIGL
MOTA	2319 O 2320 N	VAL SER	288	13.123	71.530 105.197	1.00 23.99	HIGL
MOTA MOTA	2321 CA	SER	288	12.609	71.083 104.598		HIGL
MOTA	2322 CB	SER	288	12.661	71.204 103.077	1.00 25.83	HIGL
ATOM	2323 OG	SER	288	13.511	70.204 102.537	1.00 26.10	HIGL
ATOM	2324 C	SER	288	12.606	69.606 104.969	1.00 25.73	HIGL
ATOM	2325 0	SER	288	13.655	68.951 104.917	1.00 27.44	HIGL
ATOM	2326 N	LYS	289	11.456		1.00 24.12	HIGL
MOTA	2327 CA	LYS	289	11.400		1.00 23.58	HIGT
MOTA	2328 CB	LYS	289	12.074			HIGL
ATOM	2329 CG	LYS	289	11.229	66.659 103.407		HIGL
MOTA	2330 CD	LYS	289	11.870	65.809 102.341		HIGL
ATOM	2331 CE	LYS	289	10.907			HIGL
MOTA	2332 NZ	LYS	289	9.680			HIGL
ATOM	2333 C	LYS	289	12.010			HIGL
MOTA	2334 0	LYS	289	12.135 12.415			HIGL
ATOM	2335 N	GLY	290 290	12.415			HIGL
ATOM	2336 CA 2337 C	GLY GLY	290	11.587			HIGL
ATOM ATOM	2337 C 2338 O	GLY	290	10.805		3 1.00 21.50	HIGL
MOTA	2339 N	JAV	291	11.305			HIGL
A LON	2007 11	- 4,44		-			

Fig. 2 cont.

					82	2/174			
MOTA	2340 CA	VAL.	291		10.008	66.845 1	11.013	1.00 19.00	HIGL
ATOM	2341 CB	VAL	291		9.168	65.836 1	.10.206	1.00 18.98	HIGL
ATOM	2342 CG1	VAL	291		9.040	66.301 1	108.764	1.00 18.95	HIGL
	2342 CG1 2343 CG2	VAL	291		9.816	64.471 1	10.258	1.00 19.17	HIGL
ATOM		VAL	291		9.927	66.441 1	L12.479	1.00 18.36	HIGL
ATOM	2344 C		291		B.834	66.482	13.055	1.00 18.16	HIGL
MOTA	2345 0	VAL				66.061	13 098	1.00 16.75	HIGL
ATOM	2346 N	GLY	292		11.043	65.657	114 499	1.00 15.82	HIGL
MOTA	2347 CA	GLY .	292		10.943	65.858	116 401	1.00 15.38	HIGL
MOTA	2348 C		292	•	12.114	65,838	114 000	1.00 15.70	HIGL
ATOM	2349 O	GLY	292		13.248	66.043	114.990	1.00 15.70	HIGL
ATOM	2350 N	LEU	293		11.822	65.825	110./19		HIGL
MOTA	2351 CA	LEU	293		12.842	65.963	117.757	1.00 14.98	HIGL
MOTA	2352 CB	LEU	293		13.059	67.436	118.131	1.00 14.38	
MOTA	2353 CG	LEU	293		14.200	67.697	119.131	1.00 14.97	HIGL
ATOM	2354 CD1	LEU	293		14.507	69.175	119.180	1.00 16.01	HIGL
ATOM	2355 CD2	LEU	Ż93		13.824	67.197	120.524	1.00 15.85	HIGL
ATOM	2356 C	LEU .	293		12.450	65.168	119.006	1.00 14.59	HIGL
MOTA	2357 0	LEU	293		11.367	65.356	119.559	1.00 14.50	$\mathtt{HIGL}$
•	2358 N	PHE	294		13.334	64.281	119.454	1.00 14.69	HIGL
MOTA	2359 CA	PHE	294		13.047	63.487	120.644	1.00 14.76	HIGL
ATOM			294		12.807	62.023	120.288	1.00 13.63	HIGL
MOTA	2360 CB	PHE	294		11.566	61 788	119.496	1.00 14.32	HIGL
ATOM	2361 CG	PHE			11.557	61 083	118.116	1.00 14.42	HIGL
MOTA	2362 CD1	PHE	294			61.372	120 127	1.00 14.49	HIGL
MOTA	2363 CD2	PHE	294		10.394		117.372	1.00 14.13	HIGL
MOTA	2364 CE1	PHE	294		10.395			1.00 14.10	HIGL
MOTA	2365 CE2	4	294		9.225	61.149	119.397	1.00 14:10	HIGL
ATOM	2366 CZ	PHE	294		9.224	61.344	118.017	1.00 14.44	HIGL
ATOM	2367 C	PHE	294			63.552			HIGL
ATOM	2368 Q	PHE	294		15.312	63.249	121.394	1.00 15.47	
ATOM	2369 N	TYR	295		13.778		122.897	1.00 14.13	HIGL
MOTA	2370 CA	TYR	295		14.716		124.006	1.00 13.77	HIGL
ATOM	2371 CB	TYR	295		14,199	64.993	125.065	1.00 13.42	HIGL .
ATOM	2372 CG	TYR	295		15.267		126.031	1.00 12.18	HIGL
ATOM	2373 CD1	TYR	295		15.972		125.825	1.00 11.42	HIGL
MOTA	2374 CE1	TYR	295		16.991	67.020	126.696	1.00 11.09	HIGL
MOTA	2375 CD2	TYR	295		15,602		127.131	1.00 10.29	HIGL
ATOM	2376 CE2	TYR	295		16,612	65.040	128.004	1.00 10.79	HIGL
ATOM	2377 CZ	TYR	295		17.304	66.217	127.782	1.00 10.57	HIGL
ATOM	2378 OH	TYR	295		18.317	66.569	128.640	1.00 9.73	HIGL
	2379 C	TYR	295		14.783	62.609	124.586	1.00 13.63	$\mathtt{HIGL}$
MOTA	2380 O	TYR	295		13.747		124.793	1.00 13.59	HIGL
MOTA		TRP	296		15.990		124.854	1.00 12.80	$\mathtt{HIGL}$
ATOM	2381 N		296	•	16.138		125.369	1.00 12.83	HIGL
ATOM	2382 CA	TRP			17.412		124.809	1.00 13.03	HIGL
MOTA	2383 CB	TRP	296		17.448		125.023	1.00 13.14	HIGL
ATOM	2384 CG	TRP	296		18.316		125.900	1.00 13.55	HIGL
ATOM	2385 CD2	TRP	296			57.510	125.825	1.00 13.63	HIGL
MOTA	2386 CE2	TRP	296		17.949		126.747	1.00 14.63	HIGL
ATOM	2387 CE3	TRP	296		19.369		124.460	1.00 14.08	HIGL
ATOM	2388 CD1	TRP	296		16.615	21.177	124.400	1.00 13.47	HIGL
ATOM	2389 NE1	TRP	296		16.909	56.456	124.939		HIGL
ATOM	2390 CZ2	TRP	296		18.596	55,562	126.567	1.00 13.78	
MOTA	2391 CZ3	TRP	296		20.017	57.297	127.487	1.00 13.79	HIGL
ATOM	2392 CH2	TRP	296		19.624	55.953	127.390	1.00 14.10	HIGL
MOTA	2393 C	TRP	296		16.135	60.615	126.887	1.00 12.44	HIGL
MOTA	2394 0	TRP	296		16.964	61.202	127.582	1.00 11.79	HIGL
ATOM	2395 N	GLU	297		15.190	59.811	127.376	1.00 12.90	HIGL
ATOM	2396 CA	GLU	297		15.029	59,502	128.797	1.00 12.94	HIGL
MOTA	2397 CB	GLU	297		16.061	58.455	129.199	1.00 13.78	HIGL
ATOM	2398 CG	GLU	297		15.780		128.595	1.00 14.60	HIGL
ATOM	2399 CD	GLU	297		14.616		129.271		HIGL
	2400 OE1		297		13,947		130.112	1.00 13.68	HIGL
MOTA	2400 OE1		297		14.370		128.962		HIGL
ATOM			297		15.089		129.749		HIGL
MOTA	2402 C	GLU	297		15.911		130.665		HIGL
MOTA	2403 O	GLU					129.563		HIGL
ATOM	2404 N	PRO	298		14.185	01,009	, 127.703	2.00 19.00	

Fig. 2 cont.

	•						
				. 83	1174		
MOTA	2405 CD	PRO	298	13.050		1.00 14.17	HIGL
ATOM	2406 CA	PRO	298			1.00 14.61 1.00 14.43	HIGL HIGL
MOTA	2407 CB	PRO	298			1.00 14.48	HIGL
ATOM	2408 CG	PRO	298	12.143 13.750	62.555 131.857	1.00 14.61	HIGL
	. 2409 C	PRO PRO	298 298	14.058	63.339 132.754	1.00 15.09	HIGL
MOTA	2410 O 2411 N	ALA	299	13.082	61.427 132.080	1.00 14.64	HIGL
MOTA MOTA	2412 CA	ALA	299	12.601	61.093 133.419	1.00 15.80	HIGL
MOTA	2413 CB	ALA	299	11.089		1.00 15.02	HIGL
MOTA	2414 C	ALA	299			1.00 16.15 1.00 15.99	HIGL
ATOM	2415 0	ALA	299	12.746 14.410	59.459 135.148 59.479 133.646	1.00 17.81	HIGL
ATOM	2416 N	TRP TRP	300 300	.15.115	58.361 134.269	1.00 18.35	HIGL
ATOM	2417 CA 2418 CB	TRP	300	16.003	57.672 133.238	1.00 17.62	HIGL
ATOM ATOM	2419 CG	TRP	300	16.304	56,260 133.577	1.00 17.58	HIGL
ATOM	2420 CD2	TRP	300		55.281 132.714	1.00 18.60 1.00 19.31	HIGL HIGL
MOTA	2421 CE2	TRP	300	17.067	54.105 133.479 55.283 131.369	1.00 19.31	HIGL
MOTA	2422 CE3	TRP	300	17.281 16.151	55.659 134.790	1.00 18.39	HIGL
MOTA	2423 CD1 2424 NE1	TRP TRP	300 300	16.608	54.365 134.743	1.00 18.74	HIGL
MOTA MOTA	2425 CZ2	TRP	300	17.630	52.938 132.942	1.00 19.15	HIGL
MOTA	2426 CZ3	TRP	300	17.843	54.123 130.835	1.00 18.15	HIGL HIGL
ATOM	2427 CH2	TRP	300	18.011	52.969 131.621	1.00 18.86 1.00 19.00	HIGL
MOTA	2428 C	TRP	300	15.967	58.852 135.441 58.757 135.418	1.00 19.00	HIGL
MOTA	2429 0	TRP	300 :	17.197 15.299	59.358 136.473	1.00 18.81	HIGL
MOTA	2430 N 2431 CA	ILE	301 301	15.975	59.908 137.637	1.00 18.49	HIGL
MOTA MOTA	2431 CA 2432 CB	IPE	301	14.955	60.382 138.686	1.00 18.53	HIGL
MOTA	2433 CG2	ILE	301	14.008	61.385 138.058	1.00 17.80	${\tt HIGL}$
MOTA	2434 CG1	ILE	301	14.161	59.196 139.226	1.00 20.04 1.00 21.03	HIGL
MOTA	2435 CD1	ILE	301	13.109 17.002	59.586 140.250 59.006 138.311	1.00 18.58	HIGL
MOTA	2436 C	ILE	301 301	17.002	59.499 138.851	1.00 18.75	HIGL
MOTA MOTA	2437 O 2438 N	HIS	302	16.786	57.696 138.286	1.00 18.55	HIGL
MOTA	2439 CA	HIS	302	17.741	56.781 138.907	1.00 18.79	HIGL
ATOM	2440 CB	HIS	302	17.041	55.490 139.329	1.00 18.93 1.00 18.69	HIGL HIGL
MOTA	2441 CG	HIS	302	16.222	55.629 140.573 56.523 141.587	1.00 17.82	HIGL
MOTA	2442 CD2	HIS	302 302	16.287 15.191	54.769 140.884	1.00 18.89	HIGL
ATOM ATOM	2443 ND1 2444 CE1	HIS HIS	302	14.653	55.129 142.036	1.00 17.89	HIGL
ATOM	2445 NE2	HIS	302	15.300	56.191 142.483	1.00 17.70	HIGL
ATOM	2446 C	HIS	302	18.925	56.453 137.997	1.00 19.20	HIGL HIGL
MOTA	2447 O	HIS	302	19.703	55.542 138.289 57.203 136.904	1.00 19.21 1.00 19.05	HIGL
· ATOM	2448 N	ASN	303	19.057 20.140	57.203 136.904	1.00 19.03	HIGL
MOTA	2449 CA 2450 CB	asn Asn	303 303	19.737	55.956 134.909	1.00 19.73	HIGL
ATOM ATOM	2451 CG	ASN	303	20.845	55.653 133.920	1.00 20.38	HIGL
ATOM	2452 OD1		303	22.026	55.600 134.286	1.00 20.50	HIGL HIGL
ATOM	2453 ND2		303	20.474	55.436 132.662 58.352 135.265	1.00 19.58 1.00 19.33	HIGL
MOTA	2454 C	ASN	303	20.425 20.706	58.352 133.263	1.00 19.13	HIGL
MOTA	2455 O	ASN ALA	303 304	20.760	59.414 136.071	1.00 19.41	HIGL
MOTA MOTA	2456 N 2457 CA	ALA	304	20.562	60.804 135.654	1.00 18.77	HIGL
ATOM	2458 CB	ALA	304	20.840	61.662 136.876	1.00 17.04	HIGL
MOTA	2459 C	ALA	304	21.603	61.102 134.584	1.00 18.84 1.00 19.33	HIGL HIGL
MOTA	2460 O	ALA	304	21.340	61.883 133.671 60.508 134.692		HIGL
MOTA	2461 N	ASN	305 305	22.784 23.826		1.00 18.89	HIGL
MOTA	2462 CA 2463 CB	ASN ASN	305 305	25.162		1.00 20.60	HIGL
MOTA MOTA	2463 CB 2464 CG	ASN	305	25.115	58.665 134.292	1.00 21.86	HIGL
ATOM	2465 ODI		305	24.345	58.119 135.085	1.00 23.48	HIGL HIGL
ATOM	2466 ND2	2 ASN	305	25.945		1.00 23.52 1.00 18.26	HIGL
MOTA	2467 C	ASN	305	23.448			HIGL
ATOM	2468 O	ASN	305 306	23.993 22.507			HIGL
ATOM	2469 N	LEU	300	22.50	^ -		

Fig. 2 cont.

				84/174	NEAT
MOTA	2470 CA	LEU	306	22.035 58.657 131.080 1.00 17.26 21.217 59.670 130.270 1.00 16.18	HIGL HIGL
MOTA	2471 CB	LEU	306		HIGL
MOTA	2472 CG	LEU	306	19.907 60.128 130.937 1.00 16.97 19.284 61.278 130.161 1.00 15.17	HIGL
ATOM	2473 CD1	LEU	306 306	18.937 58.954 131.024 1.00 16.01	HIGL
MOTA MOTA	2474 CD2 2475 C	LEU	306	23.156 58.076 130.216 1.00 17.50	HIGL
ATOM	2475 C 2476 O	LEU	306	23.137 58.195 128.988 1.00 17.52	HIGL
MOTA	2477 N	GLY	307	24.131 57.450 130.870 1.00 17.26	HIGL
ATOM	2478 CA	GLY	307	25.235 56.836 130.159 1.00 16.70 26.294 57.773 129.616 1.00 16.64	.HIGL HIGL
MOTA	2479 C	GLY	307		HIGL
MOTA	2480 O	GLY	307 308	27.191 57.333 128.901 1.00 16.25 26.204 59.056 129.950 1.00 16.62	HIGL
MOTA MOTA	2481 N 2482 CA	SER SER	308	27.181 60.032 129.471 1.00 17.50	HIGL
ATOM ·	•		. 308	26.477 61.300 128.987 1.00 17.40	HIGL
ATOM	2484 · OG	SER .		26.026 62.065 130.091 1.00 18.14	. HIGL
MOTA	2485 C	SER	308	28.159 60.402 130.582 1.00 17.77	HIGL HIGL
MOTA	2486 O	SER	308	28.059 59.905 131.712 1.00 18.46 29.104 61.278 130.265 1.00 17.09	HIGL
MOTA	2487 N	SER	309	29.104 61.278 130.265 1.00 17.09 30.074 61.693 131.263 1.00 17.48	HIGL
MOTA	2488 CA 2489 CB	SER SER	309 309	31.384 62.138 130.599 1.00 15.98	·· HIGL
MOTA MOTA	2490 OG	SER	309	31.196 63.287 129.794 1.00 15.84	HIGL
ATOM	2491 C	SER	309	29.485 62.818 132.118 1.00 17.77	HIGL
ATOM	2492 O .	SER	309	30.100 63.268 133.084 1.00 17.93	HIGL HIGL
MOTA	2493 N	CYS	310	28.289 63.273 131.763 1.00 18.10 27.641 64.323 132.541 1.00 18.95	HIGL
MOTA	2494 CA	CYS	310 310	27.641 64.323 132.541 1.00 18.95 26.881 63.668 133.695 1.00 18.10	HIGL
MOTA MOTA	2495 C 2496 O	CYS,	310	26.437 62.528 133.583 1.00 18.94	HIGL
ATOM	2497 CB	CYS	310	26,686 65.139 131.670 1.00 19.41	HIGL
ATOM	2498 SG	CYS	310	27.452 66.412 130.600 1.00 24.23	HIGL
	- 2499 N	ALA	311	26.733 64.392 134.798 1.00 16.72 26.061 63.873 135.986 1.00 15.09	HIGL HIGL
MOTA	2500 CA	ALA ·	311		HIGL
MOTA	2501 CB	ALA ` ALA	311 311	26.451 64.713 137.187 1.00 13.34 24.539 63.768 135.917 1.00 14.53	HIGL
MOTA MOTA	2502 C 2503 O	ALA	311	23.959 62.805 136.416 1.00 14.36	HIGL
ATOM	2504 N	ASP	312	23.893 64.755 135.308 1.00 14.02	HIGL
ATOM	2505 CA	ASP	312	22.437 64.767 135.233 1.00 14.14	HIGL
ATOM	2506 CB	ASP	312	21.888 65.569 136.414 1.00 13.88 20.417 65.338 136.647 1.00 15.05	HIGL HIGL
ATOM	2507 CG	ASP	312	20.417 65.338 136.647 1.00 15.05 19.703 64.943 135.692 1.00 16.00	HIGL
ATOM	2508 OD1 2509 OD2	ASP ASP	312 312	19.973 65.562 137.795 1.00 14.74	HIGL
ATOM ATOM	2510 C	ASP	312	21.910 65.376 133.932 1.00 14.14	HIGL
ATOM	2511 0	ASP		22.085 66.571 133.690 1.00 13.77	HIGL
ATOM	2512 N	ASN	313	21.260 64.555 133.108 1.00 14.50	HIGL HIGL
ATOM	2513 CA	ASN	313	20.684 65.016 131.845 1.00 15.03 21.177 64.160 130.672 1.00 16.08	HIGL
ATOM	2514 CB	ASN	313	21.177 64.160 130.672 1.00 16.08 22.633 64.403 130.337 1.00 18.13	HIGL
ATOM ATOM	2515 CG 2516 OD1	ASN ASN	313 313	23.069 65.544 130.228 1.00 19.71	HIGL
MOTA	2517 ND2	NZA	313	23.391 63.326 130.159 1.00 17.96	HIGL
ATOM	2518 C	ASN	313	19.159 64.947 131.889 1.00 14.73	HIGL
ATOM	2519 0	ASN	313	18.491 65.155 130.881 1.00 14.78	HIGL HIGL
ATOM	2520 N	THR	314	18.608 64.649 133.057 1.00 15.17 17.160 64.535 133.207 1.00 16.32	HIGL
MOTA	2521 CA	THR THR	314 314	17.160 64.535 133.207 1.00 16.32 16.794 63.799 134.499 1.00 16.08	HIGL
MOTA MOTA	2522 CB 2523 OG1	THR	314	17.198 64.596 135.619 1.00 16.57	HIGL
ATOM	2524 CG2		314	17.497 62.452 134.563 1.00 15.34	HIGL
ATOM	2525 C	THR	314	16.444 65.878 133.237 1.00 16.22	HIGL
ATOM	2526 0	THR	314	17.033 66.908 133.551 1.00 17.07	HIGL HIGL
ATOM	2527 N	MET	315	15.161 65.851 132.911 1.00 16.05 14.352 67.055 132.929 1.00 17.30	HIGL
ATOM	2528 CA	MET	315	14.352 67.055 132.929 1.00 17.30 13.588 67.205 131.613 1.00 17.97	HIGL
ATOM	2529 CB 2530 CG	MET MET	315 315	14.505 67.282 130.405 1.00 18.13	HIGL
ATOM ATOM	2530 CG 2531 SD	MET	315	13.637 67.606 128.894 1.00 18.76	HIGL
ATOM	2532 CE	MET	315	13.387 69.339 129.091 1.00 19.34	HIGL
ATOM	2533 C	MET	315	13.393 66.933 134.104 1.00 18.03	HIGL HIGL
ATOM	2534 O	MET	315	12.283 67.467 134.103 1.00 17.72	UIGH

Fig. 2 cont.

ATOM

MOTA

MOTA

2598 N

2599 CA

# 85/174 66.195 135.108 1.00 18.72 HIGL 13.844 316 MOTA 2535 N PHE 1.00 19.71 HIGL 66.002 136.316 13.075 316 ATOM 2536 CA PHE 1.00 20.13 HIGL 64.619 136.349 316 12.431 PHE MOTA 2537 CB HIGL 1.00 20.75 11.179 64.517 135.541 2538 CG PHE 316 MOTA 1.00 21.09 64.450 134.153 HIGL 11.232 316 ATOM 2539 CD1 PHE HIGL 1.00 19.49 9.942 64.492 136.167 2540 CD2 316 PHE MOTA 1.00 20.74 HIGL 64.359 133.402 10.065 316 ATOM 2541 CE1 PHE 64.401 135.429 1.00 19.68 HIGL 8.776 2542 CE2 316 PHE ATOM 1.00 20.74 HIGL 8.836 64.335 134.041 316 ATOM 2543 CZ PHE 66.175 137.561 1.00 20.14 HIGL 13.926 ATOM 2544 C PHE 316 1.00 21.09 HIGL 15.155 66.134 137.528 316 MOTA 2545 O PHE 66.386 138.662 66.550 139.960 67.140 140.933 1.00 20.18 1.00 20.01 HIGL 317 13.232 2546 N THR ATOM HIGL 13.836 317 MOTA 2547 CA THR 1.00 19.47 1.00 20.10 HIGL 12.783 317 2548 CB THR ATOM HIGL 13.102 68.508 141.196 317 ATOM 2549 OG1 THR 1.00 18.19 1.00 20.33 66.363 142.215 HIGL 12.710 14.271 317 2550 CG2 THR MOTA HIGL 65.161 140.408 317 MOTA 2551 C THR 1.00 20.58 HIGL 64.155 139.939 13.739 2552 0 317 THR ATOM HIGL 65.087 141.299 1.00 20.32 15.265 318 2553 N PRO MOTA 1.00 20.23 1.00 19.64 1.00 19.58 HIGL 318 66.175 141.728 PRO 16.162 2554 CD MOTA 63.793 141.791 64.187 142.743 15.740 16.859 HIGL 2555 CA PRO 318 MOTA HIGL 318 2556 CB PRO ATOM 1.00 19.55 1.00 19.76 1.00 19.67 HIGL 17.416 65.425 142.093 2557 CG PRO 318 MOTA HIGL 63.044 142.498 2558 C 318 14.615 PRO ATOM 61.841 142.739 63.772 142.827 HIGL 318 14.709 2559 O PRO ATOM 1.00 19.98 HIGL SER 319 13.551 MOTA · 2560 N 1.00 20.20 HIGL 63.195 143.504 12.403 319 . ATOM 2561 CA SER 1.00 20.64 1.00 23.02 64.147 144.578 HIGL 319 11.887 ATOM 2562 CB SER 65.119 144.016 HIGL 319 11:025 2563 OG SER ATOM 1.00 20.42 62.889 142.504 HIGL 11.291 10.263 SER 319 MOTA 2564 C HIGL 62.305 142.861 1.00 20.64 MOTA 2565 O SER 319 1.00 20.38 HIGL 11.489 63.298 141.254 320 2566 N GLYATOM HIGL 10.505 63.006 140.225 1.00 19.64 320 2567 CA **GLY** MOTA HIGL 320 320 64.119 139.765 1.00 19.52 9.585 GLY ATOM 2568 C HIGL 1.00 19.02 63.862 138.996 8.657 ATOM 2569 O GLY 1.00 18.90 1.00 19.06 HIGL 65.347 140.213 321 9.833 GLN MOTA 2570 N 66.475 139.824 67.520 140.948 HIGL 8.991 MOTA 2571 CA GLN 321 1.00 20.13 HIGL 321 8.940 GLN 2572 CB MOTA 68.811 140,564 1.00 22.26 HIGL 8.219 MOTA 2573 CG GLN 321 1.00 23.01 69.703 141.762 HIGL 2574 CD 321 7.946 GLN ATOM 1.00 25.05 HIGL 69.264 142.748 7.346 321 MOTA 2575 OE1 GLN 1.00 20.98 HIGL 70.958 141.682 2576 NE2 321 8.377 GLN ATOM 67.129 138.540 1.00 18.11 HIGL 9.477 321 MOTA 2577 C GLN 1.00 17.69 HIGL 67.520 138.428 GLN 321 10.639 2578 O ATOM 67.263 137.574 67.857 136.293 8.578 1.00 17.71 HIGL ATOM 2579 N ALA 322 1.00 17.37 HIGL ALA 322 8.938 2580 CA MOTA 1.00 16.48 1.00 17.45 1.00 19.09 HIGL 7.725 67.942 135.387 322 2581 CB ALA MOTA HIGL 69.231 136.466 9.546 2582 C ALA 322 ATOM 70.041 137.268 69.476 135.706 HIGL 9.078 322 2583 O ALA MOTA HIGL 323 323 1.00 17.15 10.601 2584 N LEU ATOM HIGL 1.00 16.94 11.305 70.743 135.720 2585 CA LEU MOTA 1.00 16.28 HIGL 70.512 135.299 323 12.755 2586 CB LEU MOTA 70.773 136.279 70.423 137.707 1.00 15.82 HIGL 13.901 323 2587 CG LEU MOTA 1.00 14.61 HIGL 13.500 15.113 323 2588 CD1 LEU ATOM HIGL 69.964 135.823 1.00 14.44 2589 CD2 323 MOTA LEU 1.00 17.93 HIGL 71.677 134.731 323 10.603 2590 C LEU MOTA 9.883 71.225 133.838 HIGL 1.00 16.70 323 LEU 2591 0 MOTA 1.00 18.92 10.811 HIGL 324 324 72.980 134.893 ATOM 2592 N SER 1.00 19.03 HIGL 73.966 134.018 SER MOTA 2593 CA 1.00 19.54 HIGL 324 10.663 75.370 134.383 MOTA 2594 CB SER 1.00 20.56 1.00 19.19 HIGL 75.478 134.241 12.069 2595 OG SER 324 MOTA HIGL 10.496 73.707 132.555 324 ATOM 2596 C SER HIGL 73.843 131.697 1.00 20.39 324 9.628 2597 O SER

Fig. 2 cont.

73.338 132.282

73.073 130.927

11.743

12.217

325

325

SER

HIGL

HIGL

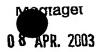
1.00 19.12

1.00 18.61

END

86/174 1.00 18.82 HIGL 72.639 130.980 13.681 325 SER 2600 CB MOTA HIGL 1.00 18.06 71.516 131.828 13.838 325 2601 OG SER ATOM 1.00 18.61 HIGL 72.047 130.132 11.414 325 SER ATOM 2602 C ·HIGL 72.036 128.905 1.00 18.45 325 11.458 2603 O SER' ATOM 71.184 130.820 70.167 130.132 1.00 19.28 HIGL 10.680 326 LEU 2604 N MOTA 1.00 19.85 HIGL 9.893 2605 CA LEU 326 MOTA 69.243 131.145 HIGL 1.00 20.13 326 9.212 LEU 2606 CB MOTA 1.00 22:13 HIGL 67.733 130.862 9.112 2607 CG LEU 326 MOTA 67.179 131.542 67.453 129.364 1.00 20.56 HIGL 7.849 326 2608 CD1 MOTA LEU 1.00 21.71 HIGL 9.063 2609 CD2 LEU 326 MOTA HIGL 1.00 20.36 70.787 129.230 326 8.822 LEU 2610 C ATOM 1.00 19.41 HIGL 70.187 128.233 8.415 2611 0 LEU 326 MOTA 71,986 129,580 1.00 20.97 HIGL 8.363 327 ATOM 2612 N SER 72.642 128.803 73.684 129.653 1.00 21.71 HIGL 7.317 327 2613 CA SER ATOM 1.00 21.54 HIGL 6.595 2614 CB SER 327 MOTA HIGL 1.00 23.10 74.785 129.921 7.439 327 2615 OG SER MOTA 1.00 22.18 HIGL 73.301 127.533 7.829 327 SER 2616 C MOTA 1.00 23.13 HIGL 74.056 126.887 7.100 327 2617 0 SER MOTA 1.00 21.90 HIGL 73.032 127.180 9.080 328 2618 N VAL MOTA HIGL 1.00 22.31 73,588 125,959 9.651 328 2619 CA VAL MOTA 1.00 22.21 1.00 21.74 HIGL 11.188 73,333 125.873 2620 CB 328 VAL ATOM HIGL 71.843 125.809 11.483 2621 CG1 328 ATOM VAL 1.00 21.78 HIGL 74.026 124.657 72.917 124.764 11.759 2622 CG2 328 VAL MOTA HIGL 1.00 22.65 328 8.958 2623 C VAL MOTA 73.429 123.645 1.00 22.63 HIGL 8.973 2624 O VAL 328 MOTA HIGL 71.771 125.013 1.00 22.73 8.338 329 2625 N PHE ATOM 1.00 23.91 HIGL 71.048 123.959 7.654 329 2626 CA PHE ATOM 1.00 23.67 HIGL 69.658 124.454 7.268 329 ATOM 2627 CB PHE 1.00 24.39 HIGL 68.723 124.557 8.440 329 2628 CG PHE ATOM 1.00 24.10 HIGL 68.252 123.409 329 9.067 2629 CD1 ATOM PHE 1.00 23.95 HIGL 68.349 125.796 8.949 PHE 329 2630 CD2 ATOM 1.00 24.86 HIGL 67.424 123.491 10.185 329 ATOM 2631 CE1 PHE HIGL 1.00 24.79 67.524 125.887 10.063 PHE 329 2632 CE2 MOTA 1.00 24.99 HIGL 67.060 124.729 329 10.686 ATOM 2633 CZ PHE 1.00 24.94 HIGL 71.806 123.420 329 6.446 2634 C PHE ATOM 1.00 24.54 HIGL 5.885 71.438 122.384 2635 O 329 PHE MOTA HIGL 1.00 25.53 72.867 124.123 330 6.053 HIS 2636 N MOTA 1.00 25.92 HIGL 4.944 73.706 123.677 330 2637 CA HIS ATOM 74.554 124.828 1.00 25.05 HIGL 4.376 330 2638 CB HIS MOTA HIGL 1.00 23.98 73.795 125.786 73.739 127.139 3.507 HIS 330 2639 CG MOTA - HIGL 1.00 23.72 3.511 2640 CD2 ·HIS 330 MOTA 1.00 23.63 HIGL 73.010 125.377 2.451 330 2641 ND1 HIS ATOM 1.00 22.96 HIGL 72.503 126.434 1.843 330 HIS 2642 CE1 MOTA 1.00 23.30 HIGL 72.931 127.517 2643 NE2 2.467 330 HIS MOTA HIGL 1.00 26.65 74.650 122.601 5.488 330 HIS ATOM 2644 C 1.00 27.30 HIGL 74.806 121.540 4.891 330 2645 O HIS ATOM 1.00 27.80 HIGL 75.267 122.888 6.632 331 ATOM 2646 N ARG 1.00 28.68 HIGL 7.273 76.214 121.976 2647 CA 331 ARG ATOM 1.00 31.32 HIGL 8.405 76.953 122.698 2648 CB ARG 331 MOTA HIGL 78.120 123.555 1.00 35.13 7.935 ARG 331 2649 CG MOTA 1.00 37.60 HIGL 78.976 124.057 9.101 2650 CD ARG 331 MOTA 1.00 39.32 HIGL 78.322 125.116 9.862 331 2651 NE ARG ATOM HIGL 1.00 41.08 9.311 7.994 77.800 126.208 77.854 126.382 2652 CZ ARG 331 ATOM HIGL 1.00 41.70 ARG 331 ATOM 2653 NH1 1.00 41.35 HIGL 10.075 77.233 127.133 MOTA 2654 NH2 ARG 331 1.00 28.01 HIGL 75.668 120.661 331 7.821 ARG ATOM 2655 C 1.00 28.33 HIGL 76,440 119.753 8.119 ARG 331 2656 O MOTA 1.00 27.15 HIGL 74.355 120.545 332 7.966 ILE MOTA 2657 N HIGL 1.00 25.82 8.503 73.790 119.313 332 2658 CA ILE **ATOM** 1.00 24.07 HIGL 72.876 119.596 9.717 332 2659 CB ILE MOTA HIGL 73.636 120.419 1.00 22.61 ILE 10.747 2660 CG2 332 ATOM 1.00 23.55 HIGL 71.611 120.331 9.262 332 2661 CG1 ILE MOTA HIGL 70.559 120.487 1.00 21.73 10.328 332 ILE 2662 CD1 MOTA HIGL 1.00 26.35 72.999 118.534 7.463 332 2663 C ILE ATOM 1.00 27.46 HIGL 72.716 117.351 7.659 MOTA 2664 O ILE 332

Fig. 2 cont.



PVS

714 <b>7</b> A	7/174			
77 77	//1 / <b>/</b>	 - 4		
		 7.7		

		87/174	PVS
			AAGL
HEADER ATOM	1 CB ALA 1	30.233 36.166 100.975	1.00 33.89 AAGL
ATOM	2 C ALA 1	30.173 35.826 103.455	1.00 33.23 AAGL
MOTA	3 0 ALA 1	30.978 35.045 103.960	1.00 32.69 AAGL
MOTA	4 N ALA 1	32.066 36.993 102.404	1.00 32.99 AAGL
MOTA	5 CA ALA 1	30.595 36.767 102.330	1.00 33.73 AAGL
ATOM	.e n ren. 5	28.909 35.906 103.856	1.00 31.18 AAGL 1.00 29.30 AAGL
MOTA	7 CA LEU 2	28.412 35.052 104.926	1.00 29.30 AAGL
MOTA	8 CB LEU 2	27.023 35.510 105.362 26.868 36.944 105.864	1.00 30.10 AAGL
MOTA	9 CG LEU 2	26.868 36.944 105.864 25.382 37.292 105.912	1.00 32.47 AAGL
ATOM	10 CD1 LEU 2 11 CD2 LEU 2	27.511 37.098 107.236	1.00 30.25 AAGL
MOTA MOTA	: 12 C LEU 2	28.340 33.612 104.451	1.00 28.19 AAGL
ATOM	13 O LEU 2	28.258 33.351 103.250	1.00 28.93 AAGL
ATOM	14 N THR 3	28.370 32.679 105.396	1.00 27.70 AAGL
ATOM	15 CA THR 3	28.304 31.267 105.071	1.00 27.25 AAGL
MOTA	16 CB THR 3	28.401 30.410 106.349	1.00 28.42 AAGL 1.00 28.17 AAGL
ATOM	17 OG1 THR 3	29.650 30.681 107.001 28.327 28.920 106.010	1.00 28.17 AAGL 1.00 27.90 AAGL
MOTA	. 18 CG2 THR · 3		1.00 26.98 AAGL
ATOM	19 C THR 3 20 O THR 3	27.000 30.971 104.343 26.965 30.159 103.416	1.00 26.10 AAGL
ATOM	20 O THR 3 21 N TYR 4	25.931 31.650 104.756	1.00 26.84 AAGL
ATOM ATOM	22 CA TYR 4	24.623 31.465 104.137	1.00 24.81 AAGL
ATOM	23 CB TYR 4	23.665 30.721 105.079	1.00 25.74 AAGL
ATOM	24 CG TYR .4	24.137 29.377 105.602	1.00 25.74 AAGL
MOTA	25 CD1 TYR 4		1.00 26.33 AAGL 1 00 27.71 AAGL
ATOM	26 CEL TYR 4	24.692 27.034 105.247	1.00 27.71 AAGL 1.00 25.74 AAGL
MOTA	27 CD2 TYR 4		1.00 25.74 AAGL
ATOM	28 CE2 TYR 4		1.00 26.22 AAGL
MOTA	29 CZ TYR 4 30 OH TYR 4		1.00 29.24 AAGL
ATOM ATOM	30 OH TYR 4		1.00 24.69 AAGL
ATOM	32 O TYR 4	23.914 33.712 104.619	1.00 24.65 AAGL
ATOM	33 N ARG 5	23.515 32.919 102.549	1.00 23.45 AAGL
ATOM	34 CA ARG 5		1.00 25.24 AAGL 1.00 29.22 AAGL
ATOM	35 CB ARG 5		
ATOM	36 CG ARG 5		
ATOM	37 CD ARG 5		
MOTA	38 NE ARG 5		
MOTA MOTA	40 NH1 ARG		1.00 27.49 AAGL
ATOM		27.068 33.068 98.104	
MOTA		21.554 33.439 101.507	
ATOM		3 21.547 32.962 100.371	
MOTA		5 20.502 33.381 102.308 6 19.321 32.694 101.837	
ATOM			
ATOM		6 18.031 33.457 101.755 6 17.957 34.649 102.053	
ATOM ATOM	<del>-</del>	7 17.008 32.727 101.330	
ATOM		7 15.669 33.248 101.182	2 1.00 22.02 AAGL
ATOM		7 15.481 33.797 99.780	1.00 22.89 AAGL
MOTA		7 14.689 32.110 101.423	
ATOM		7 14.973 30.956 101.103	
MOTA	· ·	8 13.548 32.435 102.010 8 12.501 31.448 102.24	
ATOM	•		27.07
MOTA	* -	8 11.854 31.650 103.623 8 10.772 30.617 103.923	
MOTA	<del>-</del> -	8 9.920 30.363 103.04	
ATOM ATOM		8 10.768 30.069 105.04	8 1.00 19.51 AAGL
ATOM		8 11.482 31.736 101.15	3 1.00 19.96 AAGL
ATOM		8 10.773 32.738 101.20	5 1.00 21.04 AAGL
ATOM	61 N ILE	9 11.424 30.870 100.14	9 1.00 20.91 AAGL
ATOM	62 CA ILE	9 10.490 31.065 99.04	
ATOM	63 CB ILE	9 11.234 31.102 97.68	****
MOTA	64 CG2 ILE	9 12.174 32.300 97.64 9 12.015 29.807 97.47	
MOTA	65 CG1 TLE	9 12.015 29.807 97.47	, 2.00 22.70 .2.00

Fig. 3



					88	8/174			PVS	
ATOM	. 66	CD1	ILE	9.	12.626	29.683	96.085	1.00		AAGL
ATOM	67	C	ILE	9	9.452	29.945	99.038	1.00		AAGL
ATOM	68	0	ILE	9	9.018	29.490	97.984	1.00		AAGL
MOTA	69	N	SER	10	9.059	29.511		1.00		aagl aagl
ATOM	70	CA	SER	10	8.080		100.377 101.840	1.00		AAGL
MOTA	71	CB	SER	10 10	7.658 8.782		102.658	1.00		AAGL
MOTA MOTA	72 73	og C	ser ser	10	6.833	28.617	99.508	1.00		AAGL
ATOM	74	Ö	SER	10	6.286	27.649	98.995	1.00		AAGL
MOTA	75	N	SER	11	6.388	29.855	99.347	1.00		AAGL
MOTA	76	CA	SER	11	5.198	30.148	98.563	1.00	24.59	AAGL AAGL
ATOM	77	CB	SER	11	4.784 5.775	31.598 32.473	98.792 98.275	1.00		AAGL
ATOM .	· 78 79	OG C	SER. SER	11 11	5.347	29.935	97.057		25.49	AAGL
ATOM	80	Ö	SER	11	4.351	29.913	96.338		25.69	AAGL
ATOM	81	N	LEU	12	6.578	29.781	96.583		26.51	AAGL
ATOM	. 82	CA	LEU	12	6.817	29.637	95.149		25.87	AAGL
ATOM	83	CB	LEU	12	8.237	29.143	94.884		26.84 26.26	AAGL AAGL
ATOM	84	CG	LEU	12	8.609 8.307	29.025 30.324	93.398 92.665		26.19	AAGL
ATOM	85 86		LEU LEU	12 12	10.078	28.685	93.273		28.47	AAGL
MOTA MOTA	87	C	LEU	12	5.844	28.768	94.362		28.42	AAGL
ATOM	88	Ö	LEU	12	5,181	29.257	93.447		28.84	AAGL
ATOM	89	N	LEU	13	5.758.	27.487	94.701		28.60	AAGL
MOTA	90	CA	LEU	13	4.879	26.590	93.963		30.83 30.59	AAGL AAGL
ATOM	91	CB	LEU	13	4.997 6.443	25.164 24.657	94.514 94.640		29.90	AAGL
MOTA MOTA	92 93	CG	LEU	13 · 13	6.441	23.200	95.044		30.84	AAGL
MOTA	94		LEU	13 .	7.179	24.821	93.315		31.95	AAGL
ATOM	95	C	LEU	13	3,430	27.062	93.967		31.99	AAGL
ATOM	96	0	LEU	13	2.703	26.844	93.001		33.62	AAGL
ATOM	97	N	LEU	14	3,008	27.725	95.038		33.18 33.64	AAGL AAGL
ATOM	98	ĊA	LEU	14	1.639	28.226 28.683			34.87	AAGL
ATOM ATOM	99 100	CB	LEU	14 14	1.289 0.959	27.561			35.78	AAGL
ATOM	101		LEU	14	0.492	28.145		1.00	36.41	AAGL
ATOM	102		E LEU	14	-0.137	26.693			37.20	AAGL
MOTA	103	С	LEU	14	1.423	29.385			34.86	AAGL AAGL
MOTA	104	0	LEU	14	0.352	29.522			33.97 34.48	AAGL
ATOM	105	N	LEU	15 15	2.443 2.344	30.218 31.359		•	35.10	AAGL
MOTA MOTA	106 107	CA CB	LEU	15	3.428	32.390			35.52	AAGL
ATOM	108	CG	LEU	15	3.232	33.227		1.00	37.21	AAGL
ATOM	109	CD	LEU	15	2.912	32.357			37.69	AAGL
ATOM	110	-	S TEA	15	4.496		. 94.975		35.91 35.48	. AAGL AAGL
MOTA	111	C	LEU	15	2.458	30.904 31.306			35.46	AAGL
ATOM ATOM	112 113	O N	GLU LEU	15 16	1.647 3.449	30.065		1.00	35.68	AAGL
ATOM	114	CA	GLU	16	3.619	29.561		1.00	37.14	AAGL
ATOM	115		GLU	16	4.747	28.527			35.01	AAGL
MOTA	116		GLU	16	6.159				34.68	AAGL
MOTA	117			16	7.214				35.45 35.57	AAGL AAGL
ATOM	118		1 GLU	16 16	6.928 8.336				35.12	AAGL
MOTA MOTA	119 120		2 GLU GLU	16	. 8.336 2.317				39.70	AAGL
ATOM	121		GLU	16	1.846				40.81	AAGL
ATOM	122		ASP	17	1.727				41.41	AAGL
ATOM	123			17	0.470				44.13	AAGL
ATOM	124			17	0.029				44.94	AAGL AAGL
MOTA	125			17	0.510 0.423				47.20	AAGL
MOTA	126 127		1 ASP 2 ASP	17 17	0.423				50.11	AAGL
MOTA MOTA	129		ASP	17	-0.625			1.00	45.54	AAGL
ATOM	129		ASP	17	-1.458		88.896	1.00	47.39	AAGL
MOTA	130		GLU	18	-0.629				45.43	AAGL
MOTA	131	CA	GLU	18	-1.625	30.61	7 90.234	1.00	47.08	AAGL

Fig. 3 cont.

•					. 8	9/174			
ATOM	132	CB GL	ט.	18	-1.762	31.537	91.458	1.00 49.	
ATOM	133	CG GL		18	-2.526	30.900	92.622	1.00 52.	
MOTA	134	CD GI		18	-2.530	31.755	93.890 94.911	1.00 55. 1.00 55.	65 AAGL
MOTA	135	OE1 GI		18	-3.112	31.305	93.870	1.00 56.	34 AAGL
MOTA	136	OE2 GI		18	-1.953 -1.267	32.870 31.432	88.994	1.00 46.	
MOTA	137	O GI		18 18	-1.845	32.492	88.743	1.00 46.	
MOTA	138 139	O GI		19	~0.307	30.929	88.223	1.00 45.	
ATOM ATOM	140	CA GI		19	0.091	31.609	87.006	1.00 45.	
MOTA	141	C G		19	1.245	32.588	87.113	1.00 45.	
ATOM	142		LY	19	1.636	33.185	86.113	1.00 44.	87 AAGL
ATOM	143	N T	YR	20	. 1.802	32.758	88.309	1.00 44.	
ATOM	144		YR	20	2.911	33.685		1.00 44.	
MOTA	145		YR	20	3.098	33.987 35.092	89.985 90.475	1.00 46.	
ATOM	146		YR	20 20	2.199 1.174	34.837	91.384	1.00 47.	_
MOTA	147 148	CD1 T	YR Yb	20	0.317	.35.856	91.804	1.00 48.	
MOTA MOTA	149	CD2 T		20	2.351	36.388	89.995	1.00 48.	
ATOM	150	CE2 T		20	1.509	37.406	90.399	1.00 48	
ATOM	151	CZ T	YR	20	0.494	37.135	91.301	1.00 49	.08 AAGL
MOTA	152	OH T	YR	20	~0.350	38.146	91.676	1.00 50	
MOTA	153		YR	20	4.243	33.232	87.916 87.857	1.00 42	.10 AAGL
ATOM	154		YR	20	4.541 5.040	32.043 34.211	87.494	1.00 42	
ATOM	155		ER ER	21 21	6.360	33.981	86.918	1.00 42	
ATOM ATOM	156 157		ER	21	6.255	33.775	85.402	1.00 43	
ATOM	158	-	ER	, 21	5.527	34.835	84.790	1.00 44	
ATOM	159		ER	21	7.191	35,224	87.221	1.00 41	
MOTA	160	0 8	ER	21	6.639		87.421	1.00 42	
MOTA	161.		YR	22	8.510		87.260	1.00 40	
ATOM .	162		YR	.22	9.382		87.558 88.855	1.00 40	
ATOM	163		YR	22 22	10.143 9.248	<del>-</del>	90.010	1.00 37	
MOTA	164 165	CG T	YR YP	22	8.820		90.186	1.00 35	
ATOM ATOM	166	CE1 T		22	7.987		91.246	1.00 35	
MOTA	167	CD2 7		22	8.820	36.540	90.921	1.00 37	
MOTA	168	CE2 T	'YR	22	7.982		91.982	1.00 35	
ATOM	169		CYR .	22	7.574		92.140	1.00 36	
MOTA	170		ryr	22	6.761		93.196 86.455	1.00 34	
ATOM	171		ryr Tyr	22 22	10.385 10.607		85.568	1.00 40	
MOTA	172 173		ryr Lys	· 23	10.990		86.532	1.00 40	
ATOM ATOM	174		LYS	23	11.987		85.565	1.00 41	.42 AAGL
ATOM	175		LYS	23	. 11.430		84.690	1.00 44	
ATOM	176		LYS	23	10.779		83.398	1.00 49	
MOTA	177		LYS	23	9.379			1.00 53	
ATOM	178		LYS	23	8.453		84.042 83.021		
MOTA	179		LYS	23 23	8.461 13.248				
ATOM	180 181		LYS LYS	23	13.184				
ATOM ATOM	182		ASN	24	14.39				
ATOM	183		ASN	24	15.682		_		
MOTA	184		ASN	24	16.80				
ATOM	185	CG .	ASN	24	16.73				
MOTA	186			24	16.73				
MOTA	187			24	16.67				0.98 AAGL
MOTA	188		ASN	24	15.84 14.93				
MOTA	189 190		asn Leu	24 25	16.98	-			
atom Atom	190		LEU	25	17.24			1.00 4	4.49 AAGL
ATOM	192		LEU	25	18.52			1.00 4	
ATOM	193		LEU	25	18.54	9 42.643	88.563		
ATOM	194	_		25	17.37				5.23 AAGL
ATOM	195			25	18.49				
MOTA	196		LEU	25	17.34				
ATOM	197	0	LEU	25	17.45	4 43.814	4 84.562	, 1,00 A	

Fig. 3 cont.

					90	)/174			
ATOM	198	N	ASN	26	17.311	41.675	83.880	1.00 46.41	AAGL
ATOM	199	CA	ASN	26	17.365	42.021	82.455	1.00 47.05	AAGL AAGL
ATOM	200	CB	ASN	26	18.288	41.066	81.676 82.074	1.00 47.42 1.00 49.18	AAGL
ATOM .	201	CG	ASN	26	19.747 20.207	41.198 42.276	82.459	1.00 49.93	AAGL
ATOM	202		ASN ASN	26 26	20.492	40.100	81.961	1.00 49.97	AAGL
MOTA MOTA	·203 204	C	ASN	26	15.966	41.947	81.848	1.00 47.00	AAGL
ATOM	205	ō	ASN	26	15.796	42.082	80.634	1.00 47.34	AAGL
ATOM	206	N	GLY	27	14.961	41.712	82.684	1.00 45.83	aagl aagl
MOTA	207	CA	GLY	27	13.602	41.628	82.176 81.436	1.00 45.48 1.00 45.43	AAGL
MOTA	208	C	GLY .	27 27	13.343 12.388	40.225	80.669	1.00 46.B4	AAGL
MOTA MOTA	209 210	N N	GLN	28	14.198	39.332	81.648	1.00 45.03	AAGL
MOTA	211	CA	GLN	28	14.023	38.037	81.002	1.00 44.89	AAGL
ATOM	212	CB	GLN	28	15.385	37.428	80.633	1.00 46.09	AAGL ÁAGL
MOTA	213	CG	GLN	28 .	16.346	38.371	79.909 79.531	1.00 48.72 1.00 49.91	AAGL
MOTA	214	CD	GLN GLN	28 28	17.649 17.674	37.684 36.802	78.668	1.00 51.23	AAGL
MOTA MOTA	215 _. 216		GLN	28	18.740	38.075	80.187	1.00 51.05	AAGL
ATOM	217	C.	GLN	28	13.312	37.093	81.980	1.00 43.57	AAGL
ATOM	218	o ·	GLN	28	13.800	36.871	83.088	1.00 40.72	AAGL
MOTA	219	N	THR	29	12.166	36.542	81.580	1.00 42.64 1.00 42.01	aagl aagl
MOTA	220	CA	THR	29	.11.441 10.201	35.610 35.022	82.445 81.746	1.00 42.01	AAGL
ATOM	221 222	CB OC1	THR THR	29 29	9.191	36.030	81.626	1.00 42.02	AAGL
ATOM ATOM	223		THR	29	9.639	33:857	82.552	1.00 41.97	AAGL
ATOM	224	С	THR	. 29	12.393	34.472	82.787	1.00 41.90	AAGL
MOTA	225	0	THR	29	13.233	34.095	81.966	1.00 41.33 1.00 40.58	AAGL AAGL
MOTA	226	N	GLN	30	12.261	33.909 32.835	83.984 84.392	1.00 40.38	· AAGL
ATOM	227	CA	GLN GLN	30 30	13.158 .14.585	33.383	84.396	1.00 40.50	AAGL
MOTA MOTA	228 229	CB	GLN	30	15.604	32.528	85.100	1.00 43.69	AAGL
MOTA	230	CD	GLN	30	17.014	33.031	84.892	1.00 46.36	AAGL
ATOM	231		1 GLN	30	17.325	34.200	85.159	1.00 45.16	AAGL AAGL
ATOM	232		2 GLN	30	17.888	32.145 32.268	84.409 85.763	1.00 47.79 1.00 38.44	AAGL
ATOM	233	C.	GLN GLN	30 30	12.790 12.368	33.004	86.656	1.00 38.87	AAGL
MOTA MOTA	234 235	O N	ALA	31	12.946	30.958	85.929	1.00 36.80	AAGL
MOTA	236	CA		31	12.617	30.314	87.202	1.00 34.49	AAGL
MOTA	237	CB	ALA	31	13.079	28.855	87.186	1.00 34.38 1.00 32.91	AAGL AAGL
ATOM	238	С	ALA	31	13.261	31.059 31.278	88.371 88.392	1.00 32.91	AAGL
ATOM	239	0	ala Leu	31 32	14.474 12.441	31.432	89.352	1.00 33.31	AAGL
MOTA MOTA	240	N CA		32	12.914	32.180		1.00 29.54	AAGL
ATOM	242	CB		32	11.809	32.294	91.574	1.00 28.70	AAGL
ATOM	243	CG		32	12.229	33.100	92.815	1.00 26.84	AAGL AAGL
MOTA	244		1 LEU	32	12.430	34.545 32.985	92.422 93.916		AAGL
MOTA	245		2 LEU LEU	32 32	11.173 14.160				AAGL
MOTA MOTA	246 247		LEU	32	15.068				AAGL
ATOM	248		GLU	33	14.205				AAGL
ATOM	249			33	15.360				AAGL
ATOM	250			33	15.164				AAGL AAGL
ATOM	251			33 33	15.225 13.872				AAGL
ATOM ATOM	252 253		C1 GLU	33	12.979				AAGL
ATOM	254		2 GLU	33	13.706		89.609		AAGL
ATOM	255		GLU	33	16.641				AAGL
MOTA	256	0	GLU	33	17.708				aagl aagl
MOTA	257		THR	34	16.544				AAGL
ATOM	258			34 34	17,734 17,545				AAGL
MOTA MOTA	259 260		SI THR	34	16.690			1.00 39.01	AAGL
MOTA	261		32 THR	34	16.915	28.31	87.628	1.00 33.29	AAGL
ATOM	262	. C	THR	34	18.100				AAGL AAGL
MOTA	263	3 0	THR	34	19.269	32.02	7 89.031	1.00 32.36	HUGH
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19.269 32.027 89.031 1.00 32.36 Fig. 3 cont.

					9	1/174			
ATOM	264	N	ILE	35	17.101	32.542	89.254	1.00 29.48	AAGL
ATOM	265	CA	ILE	35	17.343	33.982	89.318	1.00 29.20 1.00 29.36	aagl aagl
ATOM	266	CB	ILE	35	16.030	34.783	89.364 89.647	1.00 29.36	AAGL
ATOM	267	CG2		35 35	16.329 15.265	36.253 34.620	88.052	1.00 30.39	AAGL
MOTA MOTA	268 269	CG1	ile	35	13.998	35.456	87.981	1.00 32.09	AAGL
ATOM	270	C	ILE	35	18.103	34.276	90.605	1.00 29.48	AAGL
ATOM	271	0	ILE	35	19.039	35.068	90.627	1.00 28.30 1.00 28.93	AAGL AAGL
ATOM	272	N	LEU	36 36	17.676 18.297	33.631 33.809	91.684 92.989	1.00 28.93	AAGL
ATOM	273 274	CA CB	LEU	36 36	17.420	33.142	94.050	1.00 29.01	AAGL
ATOM ATOM	275	CG	LEU	36	16.067	33.824	94.220	1.00 29.41	AAGL
ATOM	276		LEU	36	15:139	32.993	95.105	1.00 32.23	AAGL
ATOM	277		LEU	36	16.318	35.198	94.831 93.036	1.00 29.88 1.00 26.84	AAGL AAGL
ATOM	278	C	LEU LEU	36 36	19.693 20.630	33.220 33.840	93.542	1,00 26.88	AAGL
atom atom	279 280	О И	ALA	30 37	19.829	32.005	92.515	1.00 28.77	AAGL
MOTA	281	CA	ALA	37	21.118	31.325	92.509	1.00 30.25	AAGL
MOTA	282	CB	AI.A	37	20.988	29.971	91.805	1.00 29.94 1.00 29.84	AAGL AAGL
MOTA	283	C	ALA	37 .	22.185 23.274	32.180 32.373	91.827 92.365	1.00 29.64	AAGL
ATOM ATOM	284 285	о и	ALA ASP	37 38	21.856	32.706	90.652	1.00 30.68	AAGL
ATOM	286	CA	ASP ·	38	22.798	33.524	89.894	1.00 31.88	AAGL
ATOM	287	СВ	ASP	38	22.240	33.843	88.508	1.00 32.57	AAGL
MOTA	288	CG	ASP	38	22.007	32.603	87.673 87.859	1.00 36.25 1.00 36.97	aagl aagl
ATOM	289		ASP ASP	38 38	22.749 21.085	31.610 32.621	86.830	1.00 37.38	AAGL
ATOM ATOM	290 291	C	ASP	38	23.127	34.824	90.601	1.00 31.89	AAGL
ATOM	292	ō	ASP	38	24.174	35.423	90.353	1.00 33.41	AAGL
ATOM	293	N	ALA	39	22.226	35.265	91.476	1.00 31.50 1.00 29.58	. AAGL AAGL
MOTA	294	CA	ALA	39	22.433 21.088	36.503 37.099	92.207 92.626	1.00 29.62	AAGL
ATOM ATOM	295 296	CB C	ALA ALA	39 39	23.319	36.300	93.423	1.00 29.11	AAGL
ATOM	297	Ö	ALA	39	23.739	37.268	94.053	1.00 28.08	AAGL
ATOM	298	N	GLY	40	23.603	35.047	93.769	1.00 28.38	AAGL AAGL
MOTA	299	CA	GLY	· 40	24.462	34.804 34.079	94.915 96.077	1.00 28.68 1.00 27.30	AAGL
MOTA	300 301	C	GLY GLY	40 40	23.804 24.489	33.628	96.994	1.00 28.21	AAGL
ATOM ATOM	302	Ŋ	ILE	41	22.480	33.973	96.046	1.00 27.82	AAGL
ATOM	303	CA	ILE	41	21.754	33.271	97.105	1.00 28.31	AAGL
MOTA	304	CB	ILE	41	20.231	33.267 32.678	96.841 98.047	1.00 28.86 1.00 26.11	AAGL AAGL
ATOM	305 306	CG2		41 41	19.502 19.741	34.680	96.490	1.00 32.71	AAGL
ATOM ATOM	307	CD3		41	20.041	35.739	97.526	1.00 34.86	AAGL
ATOM	308	C	ILE	41	22.262	31.830	97.055	1.00 29.05	AAGL
MOTA	309	0	ILE	41	22.275	31.223	95.982	1.00 28.58	AAGL AAGL
MOTA	310	N CA	asn asn	42 42	22.694 23.209	31.283 29.921	98.192 98.192	1.00 27.24 1.00 27.38	AAGL
MOTA ·	311 312	CB	ASN	42	24.715			1.00 26.67	AAGL
ATOM	313		ASN	42	25.014				AAGL
MOTA	314		1 ASN	42	26.177		100.422		aagl aagl
ATOM	315		2 ASN	42	23.984 22.449		100.767 99.077	1.00 28.33	AAGL
ATOM ATOM	316 317		asn Asn	42 42	22.873			1.00 25.65	AAGL
MOTA	318		SER	43	21.324			1.00 25.87	AAGL
ATOM	319			43	20.525		100.481		AAGL
ATOM	320			43	21.049		101.913		AAGL AAGL
MOTA	321			43 43	20.497 19.051		102.665 100.462		AAGL
ATOM ATOM	322 323		SER SER	43	18.714		100.411		AAGL
ATOM	324		ILE	44	18.177	27.910	100.494	1.00 24.04	AAGL
ATOM	325	CA	ILE	44	16.737		100.475		AAGL AAGL
ATOM	326			44	16.105				AAGL
ATOM ATOM	327 328		2 ILE 1 ILE	44 44	14.599 16.698				AAGL
ATOM	329		1 ILE	44	16.327				AAGL
							4		

Fig. 3 cont.

					92	2/174		
ATOM	330	С	ILE	44	16.057	27.481 101.677	1.00 23.88	AAGL
ATOM	331	0	ILE	44	16.273	26.305 101.953	1.00 22.19	AAGL AAGL
ATOM	332	N	ARG	4.5	15.244	28.262 102.384	1.00 21.15 1.00 20.84	AAGL
MOTA	333	CA	ARG	45	14.512	27.796 103.558 28.905 104.607	1.00 19.60	AAGL
ATOM	334	CB	ARG	45	14.497 13.815	28.594 105.927	1.00 22.30	AAGL
ATOM	335 336	CG CD	ARG ARG	45	13.941	29.840 106.803	1.00 22.44	AAGL
MOTA MOTA	337	NE	ARG	45	13.442	29.713 108.172	1.00 21.57	AAGL
ATOM	338	CZ	ARG	45	12.253	30.147 108.580	1.00 21.21	AAGL
ATOM	339		ARG	45	11.420	30.721 107.726	1.00 19.38	AAGL
MOTA	340	NH2	ARG	45	11.924	30.071 109.864	1.00 18.87	AAGL AAGL
ATOM	341	С	ARG	45	13.091	27.456 103.120 28.214 102.376	1.00 18.60 1.00 19.88	AAGL
ATOM	342	0	ARG .	45	12:471 12.582	26.314 103.574	1.00 19.69	AAGL
ATOM ATOM	343 344	N CA	GLN GLN	46 46	11,235	25.881 103.212		· · · AAGL
ATOM	345	CB	GLN	46	11.311	24.701 102.234	1.00 19.90 ·	AAGL
ATOM	346	CG	GLN	46	12.070	25.027 100.949	1.00 19.68	AAGL
MOTA	347	CD	GLN	46	12.093	23.880 99.946	1.00 23.43	AAGL
MOTA	348		<b>V</b>	46	12.705	23.992 98.882	1.00 26.77 1.00 21.73	aagl aagl
MOTA	. 349		GLN	46	11.429	22.777 100.278 25,467 104.445	1.00 21.73	AAGL
MOTA	350	C	GLN	46 46	10.432 10.896	24.649 105.238	1.00 18.22	AAGL
ATOM ATOM	351 352	И О	GLN ARG	47	9.233	26.023 104.601		AAGL
ATOM	353	CA.	ARG	47	8.409	25.670 105.751	1.00 18.38	AAGL
ATOM	354	СВ	ARG	47	7.414	26.792 106.095		AAGL
ATOM	355	CG	ARG	47.	6.542	27.319 104.954		AAGL
ATOM	356	CD	ARG	47	5.455	28.254 105.503		aagl aagl
ATOM	357	NE	ARG	47	4.735 5.228	28.978 104.453 30.016 103.783		AAGL
ATOM	358 359	CZ	ARG ARG	· 47 47	6.448	30.472 104.054		AAGL
ATOM ATOM	360		ARG	47	4.513	30.582 102.819		AAGL
ATOM	361	C	ARG	47	7.677	24.365 105.472	1.00 18.74	. AAGL
MOTA	362	0	ARG	47	7.101	24.183 104.403		AAGL
ATOM	363	N	VAL	48	7.710	23.458 106.445		AAGL
ATOM	364	CA	VAL	48	7.074	22.155 106.301		aagl aagl
MOTA	365	CB	VAL	48	8.109 7.488	21.023 106.490 19.677 106.130		AAGL
ATOM	366 367		VAL VAL	48 48	9.350	21.301 105.644		AAGL
ATOM ATOM	368	C	LAV	48	5.947	21.932 107.311		AAGL
ATOM	369	ŏ	VAL	48	6.166	22.027-108.517		AAGL
MOTA	370	N	TRP	49	4.748	21.647 106.80		AAGL
MOTA	371	CA		49	3.590	21.371 107.640		aagl aagl
ATOM	372	CB	TRP	49	2,382	22.168 107.16° 23.645 107.41		AAGL
ATOM	373	CG	TRP 2 TRP	49 . 49	2.525 1.608	24.673 107.024	1.00 18.82	AAGL
MOTA MOTA	374 375		2 TRP	49	2.125	25.897 107.50		AAGL
ATOM	376		3 TRP	49	0.396	24.678 106.31		AAGL
MOTA	377		1 TRP	49	3.535	24.271 108.09	1.00 17.67	AAGL
ATOM	378		1 TRP	49	3.300	25.620 108.14	9 1.00 18.03	aagl aagl
MOTA	379		2 TRP	.49	1.475	27.117 107.30		AAGL
MOTA	380		3 TRP	49 49	-0.253 0.291	25.899 106.11° 27.100 106.60		AAGL
ATOM	381 382	CH	2 TRP	49	3.306			AAGL
ATOM ATOM	383		TRP	49	3.553	19.231 106.56	3 1.00 19.96	aagl
ATOM	384	N	VAL	50	2.778	19.322 108.67	7 1.00 18.80	AAGL
ATOM	385	CA	VAL	50	2.522		6 1.00 20.11	AAGL
MOTA	386			50	2.398		1 1.00 18.82	aagl aagl
MOTA	387		1 VAL	50	2.120		6 1.00 21.34 6 1.00 21.13	AAGL
ATOM	388		2 VAL	50 50	3.695 1.340			AAGL
MOTA	389 390		VAL VAL	50 50	1.538			AAGL
ATOM ATOM	390		ASN	51	0.119			AAGL
MOTA	392			51	-1.044	17.251 107.58	5 1.00 25.51	AAGL
ATOM	393			51	-1.765	16.133 108.35	4 1.00 26.96	AAGL
ATOM	394	CG		51	-0.879	14.932 108.61	9 0.50 27.07	AAGI. AAGL
MOTA	395	00	DI ASN	51	-0.265	14.387 107.70	7 0.50 29.27	AAGU

Fig. 3 cont.

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ATOM	396	ND2	ASN	51	-0.821	14.505 109.878	0.50 28.87	AAGL
ATOM	397	C	ASN	51	-2.055	18.350 107.238	1.00 26.72	AAGL
ATOM	398	۰0	ASN	51	-3.204	18.305 107.668	1.00 27.90	AAGL AAGL
ATOM	399	И	PRO	52	-1.638	19.358 106.459	1.00 26.25	AAGL
MOTA	400	CD	PRO	52	-0.337	19.594 105.814	1.00 25.34 1.00 26.62	AAGL
ATOM	401	CA	PRO	52	-2.599	20.410 106.113	1.00 25.68	AAGL
MOTA	402	CB	PRO	52	-1.735	21.431 105.389	1.00 25.47	AAGL
MOTA	403	CG	PRO	52	-0.697	20.582 104.735 19.816 105.215	1.00 28.63	AAGL
ATOM	404	C	PRO	52	-3.690	19.112 104.254	1.00 27.01	AAGL
MOTA	405	0	PRO	52	-3.391 -4.949	20.086 105.543	1.00 29.82	AAGL
MOTA	406	N	SER	53	-4.949 -6.062	19.554 104.760	1.00 33.18	AAGL
ATOM	407	CA	SER	53	-7.394	20.100 105.281	1.00 35.65	AAGL
ATOM	408	CB	SER	53 53	-7.728	19.496 106.515	1.00 38.67	AAGL
ATOM	409	og	SER	53 53	-5.948	19.859 103.274		AAGL
MOTA	.410	C	SER	53 53	-6.284	19.019 102.434	1.00 32.67	AAGL
MOTA	411	о И	SER ASP	5 <i>3</i>	-5.469	21.053 102.949	1.00 31.58	AAGL
ATOM	412	CA	ASP	54	-5.343	21.444 101.555	1.00 31.37	AAGL
ATOM	413 414	CB	ASP	54	-5.736	22.922 101.389	1.00 33.51	AAGL
ATOM ATOM	415	CG.	ASP	54	-4.616	23.878 101.754	1.00 35.96	AAGL
ATOM	416		SP	54	-3.796	23.537 102.630	1.00 35.79	AAGL
ATOM	417		ASP	54	-4.569	24.986 101.166	1.00 38.48	AAGL
MOTA	418	C	ASP	54	-3.974	21.164 100.937	1.00 30.51	AAGL
MOTA	419	ō	ASP	54	-3.715	21.572 99.812	1.00 30.89	AAGL
ATOM	420	N	GLY	55	-3.110	20.460 101.670	1.00 31.08	AAGL
MOTA	421	CA	GLY	55	-1.790	20.102 101.161	1.00 29.00	AAGL
ATÒM	422	C	GLY	55	-0.684	21.149 101.119	1.00 28.85	AAGL
ATOM	423	0	GLY	<b>55</b>	0.475	20.829 100.834	1.00 27.57	AAGL
ATOM	424	N	SER	56	-1.028	22.399 101.398	1.00 29.06	AAGL
ATOM	425	CA	SER	56	-0.036	23.468 101.362	1.00 29.25	AAGL
ATOM	426	СВ	SER	56	-0.685	24.799 101.747	1.00 33.01	AAGL
ATOM	427	OG	SER	56	-1.603	25.222 100.746		AAGL
MOTA	428	С	SER	56	1.163	23.211 102.266		AAGL AAGL
MOTA	429	0	SER	56	1.013	22.944 103.462		AAGL
ATOM	430	N	TYR	<b>57</b>	2.350	23.282 101.673		AAGL
MOTA	431	CA	AYP	57	3.611	23.102 102.379		AAGL
ATOM	432	CB	TYR	57	3.773	24.192 103.455 25.586 102.983		AAGL
ATOM	433	CG	TYR	57	3.411 4.090	26.183 101.927		AAGL
ATOM	434		l TYR	57 57	3.733	27.448 101.457		AAGL
MOTA	435 436	CE:	2 TYR	57	2.363	26.291 103.575		AAGL
MOTA	437		2 TYR	57	1.992	27.555 103.119		AAGL
atom atom	438	CZ	TYR	57	2.687	28.130 102.049		AAGL
ATOM	439	ОH	TYR	57	2.323	29.367 101.572		AAGL
ATOM	440	Č	TYR	57	3.809	21.736 103.024		AAGL
ATOM	441	ŏ	TYR	57	4.583	21.619 103.972	1.00 22.67	AAGL
MOTA	442	N	ASP	58	3.121	20.701 102.540		AAGL
ATOM	443	ÇA		58	3.319	19.376 103.128		AAGL
ATOM	444	CB	ASP	58	2.084	18.473 102.946	1.00 27.80	AAGL
ATOM	445	CG	ASP	58	1.763	18.160 101.491	1.00 32.21	AAGL
MOTA	446	QD	1 ASP	58	2.652		1.00 30.26	AAGL
ATOM	447	OD	2 ASP	58	0.597	17.768 101.228	3 1.00 32.38	AAGL
ATOM	448	C	ASP	58	4.574			AAGL AAGL
MOTA	449	0	ASP		5.320	19.367 101.793		AAGL
MOTA	450		LEU		4.820			AAGL
MOTA	451				6.018	16.786 102.40		AAGL
MOTA	452				6.116			AAGL
ATOM	453				7.435			AAGL
ATOM	454		1 LEU		8.609			AAGL
MOTA	455	_	2 LEU		7.355 6.145			AAGL
MOTA	456		LEU		7,220			AAGL
MOTA	457		LEU Asp		7.220 5.061			AAGL
ATOM	458				5.145			AAGL
MOTA ATOM	459 460				3.850			AAGL
	460				3.557			AAGL
ATOM	401		. use		3.337			

Fig. 3 cont.

					94	1/174			
ATOM	462	OD1	ASP	60	4.518	13.547		1.00 40.6	
ATOM		OD2		60	2.365	14.000	30.00	1.00 42.6	
MOTA		С	ASP	60	5.439	17.689		1.00 30.4 1.00 28.8	
MOTA			ASP ·		6.266	17.816 18.710		1.00 28.4	
MOTA	466	N	TYR	61 61	4.761 4.944	20.088		1.00 25.6	0 AAGL
ATOM	467 468	CA CB	TYR TYR	61	4.100	21.031	99.080	1.00 25.2	
ATOM .	469	CG	TYR	61	4.182	22.508	98.723	1.00 25.1	4 AAGL
ATOM	470	CD1		61	5.283	23.286	99.095	1.00.23.8	
ATOM	471	CE1		61	5.360	24.639	98.759 98.006	1.00 24.6	-
MOTA	472	CD2		61	3.154 3.220	23.125 24.481	97.664	1.00 26.3	
MOTA	473 474	CE2	TYR TYR	61 61	4.327	25.231	98.043	1.00 25.4	S AAGL
ATOM ATOM	475	OH	TYR	61	4.403	26.565	97.687	1.00 24.8	
MOTA	476	Ç	TYR	61	6.422	20.444	98.330	1.00 26.8	
ATOM	477	0	TYR '	61	7.039	20.948	97.393 99.493	1.00 25.7	
ATOM	478	N .	ASN	62	6.992 8.388	20.159 20.458	99.493	1.00 25.4	
MOTA	479	CA	ASN	62 62	8.695		101.225	1.00 25.3	35 AAGL
MOTA MOTA	480 481	CB CG	asn Asn	62	8.316		102.009	1.00 25.6	66 . AAGL
MOTA	482		ASN	62	9.047	22.556	101.998	1.00 23.	AS AAGL
MOTA	483	ND2	ASN	62	7.159		102.666	1.00 21.1 1.00 25.1	
MOTA	484	С	ASN	62	9.355	19.629	98.899 98.596	1.00 23.	79 AAGL
MOTA	485	0	ASN	62 63	10.450	20.090 18.411	98.528	1.00 25.	
MOTA MOTA	486 487	N CA	LEU	63	9.856	17.589	97.708	1.00 27.	44 AAGL
MOTA	488	CB	LEU	63	.9.320	16.153	97.581	1.00 29.	
ATOM	489	CĠ	LEU	63	9.673	15.225	98.743	1.00 31.	
MOTA	490		ren	63	9.041	13.851	98.508 98.872	1.00 32. 1.00 32.	
ATOM	491		LEU	63 63	11.199 10.001	15.114 18.207	96.322	1.00 27.	
MOTA	492 493	C	LEU LEU	63	11.102	18.275	95.772	1.00 29:	37 AAGL
MOTA MOTA	494	N	GLU	64	8.882	18.662	95.768	1.00 28.	
ATOM	495	CA	GLU	64	8.859	19.280		1.00 30.	
MOTA	496	CB	GLU	64	7.414	19.642		1.00 32. 1.00 36.	
ATOM	497	CG	GLU	64	7.198 5.747	20.124		1.00 38.	83 AAGL
MOTA MOTA	498 499	CD.	GLU GLU	64 64	4.874	19.637	:	1.00 41.	75 AAGL
ATOM	500		GLU	64	5.464	21.565		1.00 41.	
ATOM	501	С	GLU	64	9.727	20.536		1.00 29-	
MOTA	502	0	GLU	64	10.525	20.769		1.00 27.	
MOTA	503	N	LEU	65 65	9.578 10.344	21.343		1.00 27.	
MOTA	504 505	CA CB	LEU	65 65	9.754	23.455		1.00 27	
MOTA MOTA	506	CG	LEU	65	10.420			1.00 25	
MOTA	507		1 LEU	65	10.528	25.628	95.760	1.00 24	
MOTA	508	CD	2 LEU	65	9.600			1.00 25 1.00 26	.15 AAGL
MOTA	509	C	LEU	65 65	11.824 12.677				
MOTA	510	0	LEU ALA	65 66	12.131				
MOTA MOTA	511 512	N ÇA		66	13,517				.19 AAGL
ATOM	513	CB		66	13.572				
MOTA	514	С	ALA	66	14.278				.46 AAGL
MOTA	515		ALA	66	15.479				.70 AAGL
MOTA	516		TAS	67 67	13.578 14.201				
MOTA MOTA	517 518			67	13.164			1.00 32	.68 AAGL
ATOM	519			67	12.902			1.00 36	
MOTA	520		LYS	67	11.676			1.00 38	
ATOM	521	CE		67	11.447				
MOTA	522			67	10.184				
MOTA	523		LYS LYS	67 67	14.813 15.943				
MOTA MOTA	524 525		ARG	68	14.05			3 1.00 31	49 AAGL
MOTA	526			68	14.49	7 22.52	3 91.988		
ATOM	527				13.30	23.41		3 1.00 31	.14 AAGL
					make H	^			

13.300 23.419 91.683 Fig. 3 cont.

### 95/174 22,760 1.00 33.54 AAGL 90.730 68 12.313 ARG ATOM 528 CG 1.00 32.13 23.518 90.619 AAGL 11.016 68 ATOM 529 CD ARG 90,303 1.00 31.17 AAGL ARG 11.222 24.924 530 NF. ATOM 25.763 90.002 1.00 32.92 AAGL 10.238 MOTA 531 CZ ARG 68 89.970 1.00 33.31 AAGL 25.327 NH1 ARG 68 8.985 532 MOTA AAGL 89.755 1.00 31.47 10.498 27.040 NH2 ARG 68 MOTA 533 1.00 31.54 AAGL 92.691 ARG 68 15.595 23.311 534 c MOTA 16.459 23.905 92.040 1.00 31.76 AAGL ARG 68 535 MOTA 0 1.00 28.62 AAGL 94.021 15.570 23.319 ATOM .536 N VAL 69 1.00 27.79 AAGL 16.584 24.025 94.794 69 MOTA 537 CA VAL 96.281 1.00 24.83 AAGL 24.061 16.204 MOTA 538 ÇB VAL 69 24.735 1.00 27.63 AAGL VAL 17.294 97.092 69 ATOM 539 CG1 1.00 26.08 AAGL 96.442 14.886 24.781 VAL 69 ATOM 540 ÇG2 1.00 29.09 AAGL 23.325 94.635 VAL 69 17.934 MOTA 541 C 94.458 1.00 28.64 AAGL 23.970 VAL 69 18.968 MOTA 542 O AAGL 1.00 29.15 17.908 21.998 94.711 LYS 70 MOTA 543 N 1.00 31.30 94.561 AAGL 19.108 21.187 LYS. 70 MOTA 544 CA AAGL 1.00 34.31 18.756 19.707 94.743 545 LYS . 70 ATOM CB AAGL 18.752 94.422 1.00 36.20 19.889 70 АТОМ 546 CG LYS 1.00 40.57 AAGT. 17.319 94.271 70 19.399 LYS ATOM 547 CD 1.00 41.78 AAGL 18.290 17.224 93.229 548 LYS 70 MOTA CE 1.00 42.36 AAGL 18.666 17.932 91.966 70 MOTA 549 NZ LYS 1.00 31.39 AAGL 19.693 21.403 93.159 550 LYS 70 ATOM С 1.00 31.53 AAGL 92.997 0 LYS 70 20.903 21.592 551 ATOM 1.00 30.10 AAGL 18.813 21.386 92.165 71 ATOM 552 N ALA 90.771 1.00 31.78 AAGL 19.196 21.564 553 CA ALA 71 MOTA 21.525 89.879 1.00 30.31 AAGL 71 17.957 MOTA 554 CB ALA 1.00 33.02 AAGL 22.870 90.570 71 19.949 555 С ALA ATOM AAGL 22.900 89.888 1.00 32.79 20.975 ATOM 556 0 ALA 71 1.00 32.06 AAGL 72 19.442 23.940 . 91,179 ATOM 557 N ALA 1.00 30.23 AAGL 25.257 91.071 72 20.054 ALA ATOM 558 CA 26.323 1.00 31.29 AAGL 91.463 72 19.048 ATOM 559 CB ALA 1.00 29.83 AAGL 25.389 91.915 72 21.316 560 ALA MOTA С 1.00 29.82 AAGL 26.463 91.990 21.908 ALA 72 MOTA 561 1.00 28.89 21.714 24.298 92.561 AAGL GLY 73 MOTA 562 N 1.00 30.91 AAGL 22.926 24.304 93.360 MOTA 563 CA GLY 73 AAGL 1.00 32.00 22.909 25.064 94.675 MOTA GLY 73 564 С 1.00 30.50 AAGL 23.939 25.589 95.111 ATOM 565 0 GLY 73 1.00 31.23 AAGL 95.316 ATOM 566 N MET 7.4 21.748 25.121 96.593 1.00 31.02 AAGL 21.641 25.814 74 MET MOTA 567 CA 1.00 29.51 AAGL 20,500 26.840 96.537 ATOM 568 CB MET 74 1.00 29.42 27.893 95.434 AAGL 74 20.676 MET MOTA 569 CG 1.00 28.77 AAGL 95.503 29.259 MOTA 570 SD MET 74 19.481 1.00 26.24 18.129 28.654 94.532 AAGL MET 74 ATOM 571 CE AAGL 1.00 29.72 24.768 97.681 74 21.388 ATOM 572 С MET AAGL 20.893 23.682 97.385 1.00 30.60 74 MOTA MET 573 0 25.075 98.925 1.00 28.06 AAGL. 21.750 SER 75 MOTA 574 N AAGL 1.00 25.93 575 SER 75 21.534 24.125 100.011 ATOM CA 22.454 24.426 101.202 1.00 25.27 AAGL MOTA 576 75 CB SER 1.00 24.77 AAGL 22.281 25.752 101.671 MOTA 577 OG SER 75 24.203 100.439 1.00 27.57 AAGL 20.075 ATOM 578 С SER 75 AAGL 1.00 26.04 19.343 25.089 99.997 579 SER 75 ATOM 0 19.655 23.268 101.286 1.00 25.74 AAGL ATOM 580 LEU 76 N 1.00 27.05 AAGL LEU 76 18.273 23.227 101.747 ATOM 581 CA 1.00 28.62 AAGL 76 17.602 21.941 101.268 MOTA 582 CB LEU 1.00 31.64 AAGL 21.726 101.615 16.130 LEU 76 ATOM 583 CG 22.677 100.772 1.00 29.51 AAGL 76 15.268 MOTA 584 CD1 **LEU** 1.00 32.16 AAGL 20.268 101.346 76 15.748 ATOM 585 CD2 LEU 1.00 24.07 AAGL 18.177 23.309 103.264 76 ATOM 586 С LEU 1.00 24.81 AAGL 587 LEU 76 18.890 22.619 103.985 ATOM 0 1.00 24.59 **AAGL** 17.293 24.179 103.732 TYR 77 **ATOM** 588 N 1.00 21.21 AAGL ATOM 77 17.044 24.375 105.162 589 CA TYR 1.00 21.04 AAGL 77 17.441 25.812 105.550 ATOM 590 CB TYR 1.00 22.71 AAGL 26.417 106.849 77 16.903 ATOM 591 CG TYR AAGL 25.664 107.800 1.00 20.07 77 16.207 TYR ATOM 592 CD1 AAGL 26.276 108.959 1.00 21.30 CE1 TYR 77 15.681 MOTA 593

Fig. 3 cont.

## 96/174 1.00 20.07 AAGL 27.784 107.091 17.069 77 CD2 TYR MOTA 594 AAGL 28.394 108.232 1.00 22.16 CE2 77 16.558 MOTA 595 TYR AAGL 27.646 109.159 1.00 22.47 15.863 77 CZ TYR **ATOM** 596 AAGL 28,312 110.248 1.00 21.22 15.331 77 MOTA 597 OH TYR AAGL 24.121 105.318 1,00 19.67 15.553 77 TYR ATOM 598 С 24.875 104.804 1.00 21.16 AAGL 14.730 TYR 77 MOTA 599 0 23.021 105.989 1.00 19.73 AAGL 15.217 78 LEU 600 N. MOTA AAGL 1.00 20.07 22.662 106.216 13.826 MOTA 601 CA LEU 78 21.140 106.164 1.00 20.48 AAGL 78 13.645 LEU 602 MOTA CB 1.00 24.57 AAGL 13.793 20.485 104.784 78 LEU MOTA 603 CG 18.969 104.898 1.00 25.27 AAGL LEU 78 13.633 604 CD1 ATOM 1.00 23.90 AAGL 21.067 103.833 12.750 78 MOTA 605 CD2 LEU 23.199 107.568 1.00 17.57 AAGL 606 LEU 78 13.379 C ATOM AAGL 1.00 18.99 22.891 108.599 13.980 78 ATOM 607 0 LEU 24.018 107.534 1.00 18.03 AAGL MOTA 608 N ASP 79 12.332 1.00 18.85 AAGL 11.754 24.642 108.721 79 ASP ATOM 609 CA 26.098 108.389 1.00 19.55 AAGL 11.386 MOTA 610 CB ASP 79 1.00 25.39 AAGL 79 10.593 26.785 109.493 ASP ATOM 611 CG 10.682 26.370 110.662 1.00 22.47 AAGL ASP 79 ATOM 612 OD1 1.00 27.84 AAGL 27.761 109.180 OD2 ASP 79 9.885 613 ATOM 1.00 16.61 AAGL. 10.514 23.848 109.116 ASP 79 ATOM 614 С AAGL 1.00 16.77 24.105 108.608 9.427 0 ASP 79 MOTA 615 AAGL 1.00 16.75 10.686 22,881 110.014 616 N LEU 80 ATOM 22.051 110.452 1.00 17.99 AAGL 9.573 617 CA LEU 80 ATOM AAGL 1.00 18.64 10.077 20.777 111.132 LEU 80 ATOM 618 CB 1.00 19.36 AAGL 19.918 110.385 LEU 80 11.103 ATOM 619 ĊG 1.00 20.62 AAGL 18.636 111.166 11.345 80 ATOM 620 CD1 LEU 19.605 108.986 1.00 18.29 AAGL 10.603 621 CD2 LEU 80 MOTA AAGL 1.00 18.46 22.802 111.441 LEŲ 80 8.708 MOTA 622 C 1.00 20.06 AAGL 9.162 23.121 112.529 80 MOTA 623 0. LEU 1.00 17.32 AAGL 23.086 111.071 7.464 624 N HIS 81 MOTA 1.00 16.30 AAGL 6.572 23.780 111.987 ATOM 625 CA HIS 81 1.00 15.62 AAGI: 24.525 111.223 5.475 81 ATOM 626 CB HIS 5.939 1.00 19.94 AAGL 25.810 110.612 MOTA 627 CG HIS 81 AAGL 26.167 110.093 1.00 19.51 7.137 628 CD2 HIS 81 MOTA 1.00 20.10 DAGT. 5.129 26.921 110.507 ATOM 629 ND1 HIS 81 AAGL 27.909 109.952 1.00 20.61 5.811 630 CE1 HIS 81 MOTA AAGL 1.00 20.38 27.477 109.693 7.031 ATOM 631 NE2 HIS 81 22.811 112.984 1.00 17.32 AAGL 5.939 632 HIS 81 ATOM C 1.00 18-88 AAGL 5.368 23.240 113.987 ATOM 633 0 HIS 81 AAGL 21.513 112.709 1.00 16.02 82 6.045 MOTA 634 N LEU 1.00 17.14 AAGL 20.480 113.588 5.484 82 ATOM 635 CA LEU 1.00 16.85 AAGL 6.339 20.342 114.850 LEU 82 MOTA 636 CB 1.00 20.75 AAGL 20.007 114.595 7.813 82 LEU ATOM 637 CG 1.00 18.12 AAGL 8.537 19.890 115.923 638 CD1 LEU 82 ATOM 1.00 18.95 1.00 18.59 AAGL 18.712 113.812 LEU 82 7.935 639 CD2 ATOM AAGL 20.826 113.965 4.048 ATOM 640 C TEO 82 AAGL 20.829 115.146 1.00 18.40 82 3.664 ATOM 641 0 LEU AAGL 1.00 16.93 21.109 112.930 83 3.268 ATOM 642 N SER 1.00 16.95 1.00 17.01 AAGL 21.475 113.052 83 1.868 ATOM 643 CA SER AAGL 1.757 22.914 113.569 83 ATOM 644 CB SER 1.00 17.93 AAGL 23.351 113.629 MOTA 645 OG SER 83 0.415 AAGL 1.00 18.89 21.367 111.649 1.276 83 ATOM 646 ¢ SER 21.239 110.664 1.00 19.84 AAGL 647 0 SER 83 2.011 MOTA 1.00 19.63 AAGL -0.046 21.404 111.561 84 ASP MOTA 648 N 21.317 110.275 1.00 20.59 AAGL -0.715 MOTA 649 CA ASP 84 AAGL 1.00 22.19 84 -2.107 20.695 110.421 ASP 650 CB MOTA 1.00 21.52 AAGL -2.062 19.246 110.817 ASP 84 MOTA 651 CG 1.00 23.10 AAGL 652 OD1 ASP 84 -1.025 18.597 110.572 MOTA -3.079 18.755 111.360 1.00 23.55 AAGL 84 QD2 ASP MOTA 653 1.00 21.71 AAGL 22.706 109.689 C ASP 84 -0.866 654 MOTA AAGL 22.854 108.563 1.00 21.81 -1.34084 MOTA 0 ASP 655 1.00 21.01 AAGL 23.717 110.453 -0.461 N THR 85 MOTA 656 AAGL -0.573 25.102 110.012 1.00 19.92 85 MOTA 657 CA THR 1.00 22.17 AAGL 25.670 110.370 85 -1.971 MOTA 658 CB THR AAGL -2.144 26.952 109.763 1.00 22.62 85 MOTA 659 OG1 THR

Fig. 3 cont.

ARCH ARCH ARCH ARCH ARCH ARCH ARCH ARCH						97	7/174		
AROM 661 C THR 85 0.527 25.958 110.646 1.00 19.33 AAGL AROM 662 0 THR 85 1.429 25.245 111.298 1.00 19.85 AAGL AROM 663 N TRF 86 0.454 27.276 110.450 1.00 19.81 AAGL AROM 666 CA TRF 86 1.455 28.199 110.980 1.00 17.88 AAGL AROM 665 CB TRP 86 0.454 27.276 110.450 1.00 17.88 AAGL AROM 665 CG TRF 86 0.672 30.016 103.399 1.00 18.15 AAGL AROM 666 CG TRF 86 0.672 30.016 103.399 1.00 18.15 AAGL AROM 667 CDZ TRF 86 0.672 30.016 103.399 1.00 18.75 AAGL AROM 667 CDZ TRF 86 0.672 30.016 103.399 1.00 18.75 AAGL AROM 667 CDZ TRF 86 0.523 30.649 107.201 1.00 21.95 AAGL AROM 667 CDZ TRF 86 0.523 30.649 107.201 1.00 21.95 AAGL AROM 667 CDZ TRF 86 0.523 30.649 107.201 1.00 21.95 AAGL AROM 667 CDZ TRF 86 0.553 30.044 108.226 1.00 21.00 AAGL AROM 671 CDZ TRF 86 0.563 30.004 108.226 1.00 21.00 AAGL AROM 671 CDZ TRF 86 0.563 30.004 108.226 1.00 21.00 AAGL AROM 671 CDZ TRF 86 0.563 30.004 108.226 1.00 21.00 AAGL AROM 673 CDZ TRF 86 3.556 31.004 107.508 1.00 21.00 AAGL AROM 673 CDZ TRF 86 3.556 31.004 107.508 1.00 21.00 AAGL AROM 673 CDZ TRF 86 3.556 31.004 107.508 1.00 20.30 AAGL AROM 673 CDZ TRF 86 3.556 31.004 107.501 1.00 20.30 AAGL AROM 677 CDZ TRF 86 3.556 31.004 107.501 1.00 20.30 AAGL AROM 677 CDZ TRF 86 1.727 27.998 113.302 1.00 15.66 AAGL AROM 677 N ALA 87 3.045 27.7998 113.302 1.00 17.68 AAGL AROM 678 CD AAA AROM 677 CDZ TRF 86 1.727 27.998 113.302 1.00 17.68 AAGL AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 678 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA AROM 679 CD AAA A	ATOM	660	CG2	THR	85		25.800 111.874		
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AROM 666 CB TRP 86							25.425 111.298		_
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APPLIED							29.654 110.800	1.00 17.85	AAGL
ATOM 667 CDZ TRP 86							30.016 109.399		
ATOM 669 CE3 TRP 86					86		30.427 108.382		
ATOM 670 CD1 TRP 86 -0.563 30 004 108 826 1.00 21.00 AAGL ATOM 671 NB1 TRP 86 -0.478 30 386 107.508 1.00 21.68 AGL ATOM 672 CZ2 TRP 86 1.418 31.065 106.007 1.00 19.73 AAGL ATOM 673 CZ3 TRP 86 3.556 31.041 107.151 1.00 20.30 AAGL ATOM 674 CH2 TRP 86 2.775 31.255 105.998 1.00 18.40 AAGL ATOM 675 C TRP 86 1.757 27.994 112.467 1.00 18.40 AAGL ATOM 676 O TRP 86 0.847 27.998 113.302 1.00 17.68 AAGL ATOM 676 C ALA 87 3.035 27.830 112.793 1.00 15.65 AAGL ATOM 676 C ALA 87 3.035 27.830 112.793 1.00 15.65 AAGL ATOM 678 CA ALA 87 3.035 27.830 112.793 1.00 15.65 AAGL ATOM 679 CB ALA 87 4.263 26.393 114.355 1.00 17.55 AAGL ATOM 680 C ALA 87 4.263 26.393 114.555 1.00 17.55 AAGL ATOM 681 O ALA 87 5.179 29.303 113.896 1.00 18.09 AAGL ATOM 681 O ALA 87 5.179 29.303 113.896 1.00 18.09 AAGL ATOM 683 CA ASP 88 4.276 31.855 115.604 1.00 18.94 AAGL ATOM 683 CA ASP 88 4.276 31.855 115.604 1.00 21.76 AAGL ATOM 685 CG ASP 88 2.216 31.855 115.604 1.00 21.76 AAGL ATOM 685 CG ASP 88 2.221 32.074 116.789 1.00 24.49 AAGL ATOM 687 OD2 ASP 88 2.221 32.074 117.826 1.00 21.76 AAGL ATOM 687 OD2 ASP 88 2.221 32.074 117.826 1.00 21.76 AAGL ATOM 687 OD2 ASP 88 2.221 32.074 117.826 1.00 21.76 AAGL ATOM 687 OD2 ASP 88 2.221 32.074 117.826 1.00 21.76 AAGL ATOM 689 C ASP 88 2.221 32.074 117.826 1.00 21.76 AAGL ATOM 689 C ASP 88 2.221 32.074 118.858 110.00 21.76 AAGL ATOM 689 C ASP 88 2.221 32.074 118.858 110.00 21.76 AAGL ATOM 689 C ASP 88 2.221 32.074 118.858 110.00 21.76 AAGL ATOM 689 C ASP 88 2.221 32.074 118.858 110.00 21.76 AAGL ATOM 689 C ASP 88 2.221 32.074 118.858 1.00 21.75 AAGL ATOM 689 C ASP 88 2.221 32.074 118.588 1.00 21.75 AAGL ATOM 689 C ASP 88 2.221 32.074 118.588 1.00 21.75 AAGL ATOM 689 C ASP 88 2.221 32.074 118.588 1.00 20.25 AAGL ATOM 689 C ASP 88 2.221 32.074 118.588 1.00 20.25 AAGL ATOM 689 C ASP 88 2.221 32.074 118.588 1.00 20.25 AAGL ATOM 689 C ASP 88 2.221 32.074 118.588 1.00 20.25 AAGL ATOM 699 C ASP 88 2.221 32.074 118.588 1.00 20.25 AAGL ATOM 699 C ASP 89 2.909 31.881 118.588 1.00 20.25 AAGL ATOM 699 C ASP 99 3.280 32.381 33							30.649 107.209		
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7 TO THE 114 OLG 1 ON 10 E1 DAGE.								1.00 23.34	
									AAGL

Fig. 3 cont.

98/174 0.000 21.935 115.856 1.00 19.99 AAGL 726 THR 93 MOTA 0 21.050 117.802 1.00 19.55 AAGL -0.685 THR ATOM 727 N 1.00 20.32 AAGL -0.181 .19.716 117.510 94 ATOM 728 CA THR 18.775 118.699 AAGL 1.00 20.34 -0.463 THR 94 ÇB MOTA 729 AAGL 1.00 20.72 19.190 119.824 94 0.320 ATOM 730 OG1 THR AAGL 17.334 118.348 1.00 20.41 94 -0.141CG2 THR ATOM 731 AAGL 1.00 19.20 -0.866 19.171 116.261 94 THR ATOM 732 C 19.367 116.071 AAGL 1.00 19.04 -2.060 733 0 THR 94 MOTA 1.00 19.53 AAGL 18.495 115.381 -0.111 95 734 MOTA N PRO 1.00 17.38 AAGL 1.352 18.315 115.386 MOTA 735 CD PRO 95 AAGL 1.00 20.73 17.937 114.160 PRO 95 -0.703CA MOTA 736 1.00 16.98 AAGL 17.086 113.590 0.424 95 ATOM 737 CB PRO AAGL 17.872 113.952 1.00 20.07 PRO 95 1.638 736 CG MOTA 1.00 22.21 AAGL 17.091 114.452 95 -1.939PRO 739 С MOTA 1.00 19.37 AAGL -2.002 -2.926 16.399 115.468 740 o. PRO 95 MOTA AAGL 1.00 23.26 17.163 113.569 96 SER ATOM 741. N AAGL 1.00 27.34 16.353 113.740 -4.125 MOTA 742 CA SER 96 1.00 29.38 AAGL 16.695 112.656 СВ 96 -5.153 SER ATOM 743 AAGL 16.561 111.365 1.00 34.62 -4.577 SER 96 MOTA 744 OG AAGL 1.00 28.07 -3.635 · 14.911 113.590 SER 96 745 C ATOM AAGL 1.00 29.54 . -2.863 14.602 112.685 96 746 0 SER **ATOM** 14.029 114.482 1.00 28.91 AAGL 97 -4.064 MOTA 747 N GLY 1.00 28.58 AAGL -3.60712.655 114.390 GLY 97 ATOM 748 CA 12.365 115.365 1.00 27.25 AAGL -2.478 97 MOTA 749 C GLY AAGL 1.00 28.56 11.202 115.679 GLY 97 -2.214 750 0 ATOM AAGL .13.408 115.819 1.00 23.62 -1.786TRP 98 ATOM 751 N 1.00 20.63 AAGL 13.227 116.801 -0.715 TRP 98 752 CA MOTA AAGL 1.00 20.68 0.396 14.250 116.590 753 CB TRP 98 ATOM 13.995 115.382 1.00 20.26 AAGL 1.253 ATOM 754 CG TRP 98 1.00 19.57 AAGL 14.517 115.148 2.561 98 MOTA 755 CD2 TRP AAGL 14.123 113.845 1.00 20.94 2.945 756 CE2 TRP 98 ATOM 1,00 19.61 AAGL 15.288 115.913 98 3.449 CE3 TRP ATOM 757 AAGL 0.905 13.311 114.246 1.00 21.24 CD1 TRP 98 MOTA 758 1.00 21.31 AAGL 13.386 113.318 1.918 759 NE1 TRP 98 ATOM AAGL 1.00 20.47 4.178 14.475 113.290 760 CZ2 TRP 98 ATOM 15.638 115.362 1.00 20.55 AAGL 4.675 CZ3 TRP 98 ATOM 761 AAGL 1.00.21.24 15.230 114.05B CH2 TRP 5.028 ATOM 762 98 1.00 21.31 AAGL 13.397 118.190 -1.348 98 763 TRP . ATOM C 1.00.21.68 AAGL -2.422 13.973 118.312 TRP 98 ATOM 764 0 AAGL 12:910 119.227 1.00 22.27 -0.675 ATOM 765 N SER 99 1.00.20.04 AAGL 12.951 120.591 -1.210 99 766 CA SER MOTA AAGL 11.870 121.446 1.00 21.78 -0.531 767 SER 99 MOTA CB AAGL 11.794 122.746 1.00 19.99 -1.115SER 99 MOTA 768 OG 1.00 20.81 AAGL 14.262 121.377 -1.172 99 769 С SER ATOM -0.174 14.974 121.391 1,00 20,17 AAGL 99 770 SER 0 ATOM 1.00 21.47 AAGL -2.284 14.555 122.039 THR 100 MOTA 771 N AAGL 15.730 122.896 1.00 22.60 -2.401 THR 100 ATOM 772 CA AAGL 1.00 22.41 16.655 122.455 -3.564THR 100 ATOM 773 CB AAGL 1.00 23.06 15.882 122.308 -4.759 100 774 OG1 THR MOTA AAGL 17.339 121.128 1.00 22.11 -3.248CG2 THR 100 775 ATOM 1.00 23.80 AAGL -2.706 15.190 124.294 776 С THR 100 ATOM 1.00 23.03 AAGL -3.150 15.930 125.174 THR 100 777 0 ATOM -2.448 -2.737 1,00 24.54 AAGL 13.895 124.488 778 N THR 101 ATOM 1.00 23.47 AAGL 13.228 125.755 CA THR 101 779 MOTA AAGL -4.055 1.00 24.48 12.440 125.638 MOTA 780 CB THR 101 AAGL 1.00 25.27 -3.897 11.412 124.652 THR 101 781 OG1 MOTA 1.00 25.93 AAGL -5.198 13.356 125.213 101 CG2 THR MOTA 782 AAGT. 1.00 25.35 -1.679 12.256 126.301 THR 101 ATOM 783 C AAGL 1.00 25.05 -1.794 11.802 127.437 101 0 THR 784 ATOM AAGL 11.932 125.513 1.00 23.02 -0.657 ATOM 785 N ASP 102 1.00 24.03 AAGL 0.366 10.989 125.968 ASP 102 786 CA **ATOM** AAGL 1.00 25.87 0.013 9.579 125.488 MOTA 787 СВ AS2 102 1.00 29.80 8.515 126.052 AAGL 0.934 788 CG ASP 102 MOTA 1.00 30.75 AAGL 8.600 125.864 2.163 102 OD1 ASP ATOM 789 AAGL 1.00 35.27 7.571 126.683 0.425 790 OD2 ASP 102 MOTA AAGL 1.00 24.10 11.370 125.446 102 MOTA 791 С ASP 11.269 124.245 1.00 24.23 AAGL 2.005 ATOM 792 0 ASP 102

Fig. 3 cont.

					99	9/174		
ATOM	793	N	LEU	103	2.640	11.791 126.338	1.00 23.33	AAGL
ATOM	794	CA	LEU	103			1.00 23.77	aagl aagl
ATOM	795	CB	LEU	103	4.801		1.00 24.26 1.00 23.41	AAGL
MOTA	796	CG	LEU	103	6.113	13.383 126.579 14.627 125.765	1.00 23.41	AAGL
ATOM		·CD1		103 103	5.800 7.005	13.729 127.764	1.00 24.01	AAGL
ATOM ATOM	798 799	CD2 C	FEO	703	4.744	11.046 125.257	1.00 24.93	AAGL
ATOM	800	õ	LEU	103	5.522	11.259 124.326	1.00 22.87	AAGL
ATOM	801	N	GLY	104	4.535	9.837 125.765	1.00 24.55	AAGL .
MOTA	802	CA	GLY	104	5.229	8.689 125.213	1.00 25.67 1.00 24.34	aagl aagl
MOTA	803	Ç	GLY	104	4.863	8.514 123.757 8.334 122.699	1.00 24.34	AAGL
ATOM	804	0	GLY	104	5.727 3.571	8.571 123.475	1.00 23.72	AAGL
ATOM	805 806	N CA	THR THR	105 105	3.084	8.425 122.115	1.00 24.93	AAGL
ATOM ATOM	807	CB	THR	105	1.546	8.360 122.095	1.00 25.14	aagl
ATOM	808		THR	105	1.109	7.236 122.870	1.00 28.55	AAGL
ATOM	809	CG2	THR	105	1.029	8.211 120.684	1.00 27.78	aagl aagl
MOTA	810	С	THR	105	3.561	9.596 121.260 9.412 120.132	1.00 23.97 1.00 24.40	AAGL
ATOM	811	0	THR	105	4.,008 3.485	10.802 121.812	1.00 22.92	. AAGL
ATOM	812	N	LEU LEU	106 106	3.898	12.000 121.085	1.00 21.38	AAGL
MOTA MOTA	813 814	CA CB	LEU	106	3.568	13.254 121.896	1.00 19.99	AAGL
ATOM	815	CG	LEU	106	3.895	14.579 121.196	1.00 18.13	AAGL
MOTA	816		LEU	106	3.066	14.714 119.923	1.00 16.54	AAGL ·
ATOM	817		LEU	106	3.613	15.735 122.141	1.00 15.43 1.00 23.00	AAGL AAGL
ATOM	818	C	LEU	106	5.382	11.995 120.729 12.330 119.601	1.00 23.00	AAGL .
MOTA	819	0	LEU LYS	106 107	5.755 6.230	11.627 121.684	1.00 23.39	AAGL
ATOM ATOM	820 821	N CA	LYS	107	7.662	11.578 121.420	1.00 24.69	AAGL
ATOM	822	CB	LYS	107	8.446	11.129 122.660	1.00 25.78	. AAGL
ATOM	823	ÇG	LYS	107	8.496	12.144 123.789	1.00 27-94	AAGL
MOTA	824	CD	LYS	107	9.574	11.781 124.801	1.00 31.83	AAGL AAGL
MOTA	825	CE	LYS	107	9.360	10.393 125.384 10.009 126.355	1.00 36.44 1.00 39.34	AAGL
ATOM	826	ΝZ	LYS	107 107	10.431 7.942	10.609 120.278	1.00 24.60	AAGL
MOTA MOTA	827 828	C	LYS LYS	107	- 8.829	10.852 119.461	1.00 24.29	AAGL
ATOM	829	И	TRP	108	7.183	9.518 120.220	1.00 24.58	AAGL
ATOM	830	CA	TRP	108	7.372	8.526 119.165	1.00 26.57	AAGL
ATOM	831	СВ	TRP	108	6.616	7.231 119.487	1.00 30.79 1.00 37.55	AAGL AAGL
ATOM	832	CG	TRP	. 108	7.429	6.243 120.257 5.579 119.806	1.00 37.33	AAGL
ATOM	833		TRP TRP	108 108	8.617 9.055	4.744 120.861	1.00 41.70	AAGL
MOTA MOTA	834 835		TRP	108	9.356	5.610 118.611	1.00 40.79	AAGL
ATOM	836		TRP	108	7.199	5.797 121.530	1.00 39.67	AAGL
ATOM	637		1 TRP	108	8.173	4.898 121.899	1.00 41.76	AAGL
MOTA	838		Z TRP	108	10.202	3.942 120.760	1.00 42.41 1.00 42.96	AAGL AAGL
MOTA	839		3 TRP	108	10.498	4.814 118.510 3.992 119.582	1.00 42.90	AAGL
ATOM	840		2 TRP	108 108	10.908 6.925	9.040 117.807	1.00 25.36	AAGL
MOTA MOTA	841 842	C	TRP TRP	108	7.585	8.785 116.801	1.00 25.01	AAGL
ATOM	843		GLN	109	5.808	9.763 117.782	1.00 22.63	AAGL
MOTA	844			109	5.277	10.304 116.539	1.00 22.94	AAGL
MOTA	845	CB		109	3.884	10.886 116.784	1.00 22.73 1.00 24.36	AAGL AAGL
MOTA	846			109	2.863			AAGL
MOTA	847			109 109	1.555 1.551		1.00 25.25	AAGL
MOTA	848 849		1 GLN 2 GLN	109	0.434			AAGL
ATOM ATOM	850		GLN	109	6.212	11.362 115.958	1.00 22.81	AAGL
ATOM	851		GLN	109	6.416	11.418 114.747	1.00 23.48	AAGL
MOTA	852		LEU	110	6.796			AAGL
ATOM	853			110	7.716			AAGL AAGL
ATOM	854			110	8.031	14.188 117.539		AAGL
MOTA	855		,	110	9.119 8.792			AAGL
ATOM ATOM	856 857		1 LEU 2 LEU	110 110	9.230		1.00 23.11	AAGL
ATOM	858		LEU	110	9.005		1.00 25.82	AAGL
ATOM	859		LEU	110	9.523			AAGL

9:523 13:010 114:835 Fig. 3 cont.

						VIIIT				
MOTA	860	N T	YR	111		11.608 1	16.594		25.68	aagl aagl
MOTA	861		YR	111		10.915 1	17 270		24.78 25.83	AAGL
ATOM	862		'YR	111	11.151	9.869 1			27.35	AAGL
atom	863		ryr	111	12.199	8.874 I			29.55	AAGL
ATOM	864	CD1		111	11.848	6.866	15 544		31.93	AAGL
MOTA	865	CE1 7		111	12.810 13.541	9.043			28.41	AAGL
ATOM '	000	CD2		111 111	14.514	8,143			32.12	AAGL
ATOM .	867		ryr ryr	111	14.143	7.060			31.55	AAGL
MOTA	868 869		TYR TYR	111	15.104		L15.423		34,00	AAGL
MOTA MOTA	870		TYR	111	10.505	10.246		1.00	24.33	AAGL
ATOM	871		TYR	111	11.307	10.383		1.00	26.25	AAGL
ATOM	872		AŞN	112	9.398	9.521	114.731		23.20	AAGL
MOTA	873		ASN	112	9.042		113.492		24.57	AAGL
ATOM	874	CB .	ASN	112	. 7.750	8.041			27.15	AAGL
MOTA	875	CG .	ASN	112	7.963		114.473		25.91	AAGL AAGL
MOTA	876	OD1		112	7.010		114.752		29.07 26.44	AAGL
MOTA	877	ND2		112	9.209		114.825		26.29	AAGL
MOTA	878		ASN.	112	8.865	-	112.364 111.211		23.16	AAGL
MOTA	879		ASN	112	9.227 · 8.317	11.028			23.87	AAGL
MOTA	880		TYR.	113	8.097	12.075			23.73	AAGL
MOTA	881		TYR	113 113	7.328	13.239			23.08	AAGL
ATOM	882 883	CB CG	TYR TYR	113	7.148	14.387			22.30	AAGL
MOTA MOTA	884	CD1		113		. 14.271		1.00	20.43	AAĢL
MOTA	885	CE1		113	6 134		109.335	1.00	21.15	AAGL
ATOM	886	CD2		113	7.847	15.584	111.510		20.85	AAGL
ATOM	887	CE2		113	7.699		110.612	_	18.32	AAGL
ATOM	888	CZ	TYR	113	6.846		109.533		19.02	AAGL
MOTA	889	OH	TYR	113	6.706		108.654		18.05	AAGL
ATOM	890	С	TYR	113	9.391		111.111		23.40	aagl aagl
MOTA	891	0	TYR	113	9.561		109.891		24.13 22.35	AAGL
MOTA	892	N	THR	114	10.300		111.957 111.441		23.52	AAGL
ATOM	893	CA	THR	114	11.552 12.413		112.569		22.78	AAGL .
ATOM	894	CB OG1	THR	114 114	12.714		113.578		23.02	AAGL
MOTA	895 896		THR	114	11.662		113.210		22.56	AAGL
MOTA MOTA	897	, CG2	THR	114	12.339		110.711	1.00	24.38	AAGL
ATOM	898	ŏ	THR	114	12.954	12.783	109.673	1.00	23.70	AAGL
ATOM	899	N	LEU	115	12.309	11.315	111.250		26.01	AAGL
MOTA	900	CA	LEU	115	12.995		110.618		26.48	AAGL
MOTA	901	CB	LEU	115	12.785		111 - 443		27.61	AAGL
ATOM	902	CG	TEA	115	13.278		110.853	1.00	28.64	AAGL
MOTA	903		LEU	115	14.787		110.546		0 29.41	AAGL AAGL
ATOM	904		LEU	115	12.991		111.836		0 31.02	AAGL
MOTA	905	C	LEU	115	12.432		109.208 108.236		0 29.69	AAGL
ATOM	906	0	LEU	115	13.180 11.106		109.102		0 27.14	AAGL
ATOM	907 908	N	GLU GLU	116 116	10.428		107.825		0 28.85	AAGL
MOTA MOTA	909	CA CB	GLU	116	8.919	9.674	108.057		0 33.11	AAGL
ATOM	910	CG	GLU	116	8.111		106.803	1.0	0 40.59	AAGL
ATOM	911	CD	GLU	116	8.196		106.368		0 44.26	AAGL
ATOM	912		GLU	116	7.696	7.603	105.266	1.0	0 47.23	AAGL
MOTA	913		GLU	116	8.744	7.073	107.118	1.0	0 47.05	AAGL
ATOM	914	С	GLU	116	10.707	10.952	106.853		0 28.50	AAGL
ATOM	915	0	GLU	116	10.936		105.667		0 28.60	AAGL
ATOM	916	N	VAL	117	10.671	12.184	107.354		0 25.75	AAGL
MOTA	917	CA	VAL		10.933		106.507		0 25.01	AAGL
ATOM	918	CB	VAL		10.841		107.303		0 25.08	AAGL AAGL
ATOM	919		VAL		11.393		106.473		0 24.84	AAGL
ATOM	920		VAL		9.390		107.685 105.894		0 25.17	AAGL
MOTA	921		VAL		.12.321		105.894 104.684		0 25.19	AAGL
MOTA	922		VAL		12.488 13.313		104.004	_	0 22.94	AAGL
ATOM	923		CYS		14.684		106.261		0 24.56	AAGL
MOTA MOTA	924 925		CYS		15.644	12.710	107.446		0 24.73	AAGL
ATOM	925		CYS		15.852		108.485	_	0 26.92	AAGL
WION	720	39	~ 13	F 7. C	20.002					

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አም <b>ሶ</b> ል	927	C	CYS	118	14.810	11.682	105.289	1.00	25.33	AAGL
ATOM ATOM	928		CYS	118	15.417	11.813	104.228	1.00		AAGL
ATOM	929		ASN	119	14.224	10.537		1.00		AAGL
ATOM	930	CA .	ASN	119	14.296		104.753	1.00	28.13 28.39	AAGL AAGL
ATOM	931		ASN	119	13.618	8.150	105.382 106.477	•	28.84	AAGL
ATOM	932		ASN	119	14.446 15.607		106.681		28.82	AAGL
MOTA	933 934	OD1 ND2		119 119	13.858		107.191		31.56	AAGL
ATOM ATOM	935		ASN	119	13.685		103.381	1.00	28.08	AAGL
MOTA	936		ASN	119	14.199		102.376		31.49	AAGL
ATOM	937	N	THR	120	12.594	10.372	103.326		28.01	aagl aagl
ATOM	938		THR	120	11.952	10.641	102.046		27.89 30.29	AAGL
ATOM	939	CB	THR	120	· 10.596 9.752	10.490	102.231 103.034		31.43	AAGL
ATOM	940	OG1 CG2:		120 120	9.926		100.873		30.28	AAGL
ATOM ATOM	941 942	CGZ.	THR	120	12.838		101.147		28.78	AAGL
ATOM	943	0	THR	120	12.869	11.290	99.933		29.09	AAGL
ATOM	944	Ŋ	PHE	121	13.557	12.452	101.728		28.45	AAGL
ATOM	945	CA	PHE	. 121	14.463	13.269	100.930		28.19	aagl aagl
MOTA	946	CB	PHE	121	14.985		101.741		29.04 27.88	AÄGL
MOTA	947	CG	PHE	.121	14.023 12.847		102.530		28.91	AAGL
MOTA	948	CD1 CD2		121 121	14.242	16.753	101.018		28.77	AAGL
MOTA MOTA	949 950	CE1		121	11.905		102.496	1.00	26.83	AAGL
ATOM	951		PHE	121	13.301	17.780	100.979		29.21	AAGL
ATOM	952	CZ	PHE	121	12.130		101.719		29.40	AAGL
ATOM	953	С	PHE	121	15.622		100.454		28.62	AAGL AAGL
ATOM	954	0	PHE	121	16.064	12.485	99.308	1.00	29.15 28.34	AAGL
MOTA	955	N	ALA	122	16.102 17.187		101.332 100.964	1 00	29.64	AAGL
MOTA	956	CÁ	ALA ALA	122 122	17.599		102.158	1.00	27.49	AAGL
MOTA MOTA	957 958	CB C	ALA	122	16.748	9.731	99.795	1.00	29.44	AAGL
ATOM	959	Ö	ALA	122	17.538	9.447	98.890		30.54	AAGL
ATOM	960	N	GLU	123	15.492	9.295			27.94	AAGL
ATOM	961	CA	GLU	123	15.004	8.448	98.720		28.60	AAGL AAGL
ATOM	962	CB	GLU	123	13.654	7.837	99.085 100.439		30.65 35.94	AAGL
ATOM	963	CG	GLU	123 123	13.693 12.401		100.433		38.73	AAGL
ATOM ATOM	964 965	CD OE1	GLU GLU	123	11.315		100.376		39.11	AAGL
ATOM	966		GLU	123	12.485		101.570	1.00	39.90	AAGL
ATOM	967	C	GLŲ	123	14.899	9.237			28.83	AAGL
ATOM	968	0	GLU	123	14.826	8.658			25.94	AAGL AAGL
MOTA	969	N	ASN	124	14.893	10.561			27.22	AAGL
MOTA	970	CA	ASN	124 124	14.825 13.786	11.434 12.537			27.25	AAGL
MOTA MOTA	971 972	CB CG	ASN ASN	124	12.367	12.067			28.47	AAGL
ATOM	973		ASN	124	11.888	12.130	95.168		28.23	AAGL
ATOM	974		ASN	124	11.691	11.580		1.00	30.75	AAGL
MOTA	975	С	ASN	124	16.186	12.063			26.40	AAGL AAGL
ATOM	976	0	ASN	124	16.290	13.015			25.52	AAGL
MOTA	977	N	ASP	125	17.223	11.538 12.039			29.66	AAGL
ATOM	978	CA CB	ASP ASP	125 125	18.580 19.066	11.654			31.58	AAGL
MOTA MOTA	979 980		ASP	125	20.550	11.898			34.86	AAGL
ATOM	981		ASP	125	21.314	11.723		1.00	36.55	AAGL
ATOM	982		ASP	125	20.958	12.254			35.76	AAGL
MOTA	983	C	ASP		18.715	13.555	<b>.</b>		30.52	AAGL
ATOM	984		ASP		19.286	14.265		_	0 28.80 0 30.01	AAGL AAGL
ATOM	985		ILE		18.181	14.042			0 30.54	AAGL
ATCM	986		ILE		18.270 16.886	15.458 16.127			0 30.36	AAGL
ATOM ATOM	987 988		ILE ILE		17.014	17.532	_		0 31.24	AAGL
MOTA	989		LILE		16.294	16.182		1.0	0 29.46	
MOTA	990		LILE		14.803		96.798	1.0	0 32.42	AAGL
ATOM	991		ILE	126	18.894				0 32.08	
ATOM	992		ILE		18.381		3 100.550		0 33.29	
ATOM	993	N	ASP	127	20.004	16.292	2 99.689	1.0	0 30.97	MMGD

Fig. 3 cont.

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ATOM	994	CA	ASP	127		16.475 100.960	1.00 32.32	AAGL
ATOM	995		ASP	127		16.777 100.719	1.00 36.39 1.00 40.70	AAGL AAGL
ATOM.	996		ASP	127		15.758 99.822 14.591 100.244	1.00 43.54	AAGL
MOTA	997	OD1		127 127	23.019 23.201	16,126 98.680	1.00 45.38	AAGL
MOTA	998 999	OD2 C	ASP ASP	127	20.082	17.655 101.687	1.00 31.14	AAGL
ATOM ATOM	1000		ASP	127	19.643	18.616 101.053	1.00 30.94	AAGL
ATOM	1001	N	ILE	128	20.063	17.587 103:012	1.00 29.03	AAGL
MOTA	1002	CA	ILE	128 -	19.505	18.659 103.825	1.00 27.70	AAGL
ATOM	1003	CB	ILE	128	18.442	18.112 104.806	1.00 27.94	AAGL
ATOM	1004	CG2	ILE	128	17.866	19.250 105.645	1.00 25.95 1.00 27.55	aagl aagl
MOTA	1005		ILE	128	17.333 16.289	17.408 104.017 16.716 104.883	1.00 27.33	AAGL
ATOM	1006	CD1	ILE	128 128	20.630	19.317 104.611	1.00 25.60	AAGL
ATOM ATOM	1007 1008	C O	ile Ile	128	21.370	18.645 105.328	1.00 28.07	AAGL
ATOM	1009	N	GLU	129	20.766	20.632 104.465	1.00 24.98	AAGL
ATOM	1010	CA	GLU	129	21.818	21.380 105.156	1.00 24.49	AAGL
ATOM	1011	CB	GLU	129	22.107	22.671 104.382	1.00 27.35	AAGL
ATOM	1012	CG	GLU	129	23.218	23.552 104.946	1.00 30.16 1.00 32.15	AAGL AAGL
ATOM	1013	CD	GLU	129		22.996 104.682 22.097 103.821	1.00 32.13	AAGL '
MOTA	1014		GLU	129 129	24.720 25.563	23.469 105.326	1.00 31.39	AAGL
MOTA MOTA	1015 1016	C	GLU GLU	129	21.418	21.713 106.593	1.00 24.14	AAGL
MOTA	1017	ò	GLU	129	22.210	21.561 107.531	1.00 23.23	AAGL
ATOM	1018	N	ILE	130	20.184	22.174 106.761	1.00 22.11	AAGL
MOTA	1019	CA.	ILE	130	19.696	22.535 108.083	1.00 20.15	AAGL
MOTA	1020	CB	ILE	130	19.719	24.065 108.301	1.00 21.07 1.00 22.31	AAGL AAGL
MOTA	1021		ILE	130	19.096 21.147	24.406 109.636 24.601 108.233	1.00 20.04	AAGL
ATOM	1022		ILE	130 130	21.147	26.109 108.266	1.00 20.01	AAGL
ATOM	1023 1024	C	ILE	130	18.256	22.091 108.265	1.00 20.32	AAGL
MOTA MOTA	1025	Ö	ILE	130	17.464	22.096 107.328	1.00 18.94	AAGL
ATOM	1026	N	ILE	131	17.920	21.696 109.480	1.00 21.44	AAGL
ATOM	1027	ÇA	ILE	131	16.551	21.316 109.759	1.00 22.36	AAGL
ATOM	1028	СВ	ILE	131	16.324	19.791 109.544	1.00 23.90	AAGL
MOTA	1029		ILE	131	17.138	18.979 110.541 19.488 109.629	1.00 28.54 1.00 26.48	aagl aagl
MOTA	1030	CG1		131 131	14.826 14.427	18.156 109.005	1.00 28.03	AAGL
ATOM ATOM	1031 1032	C	ILE	131	16.253	21.765 111.185	1.00 21.53	AAGL
MOTA	1033	ŏ	ILE	131	16.978	21.430 112.119	1.00 20.84	AAGL
ATOM	1034	N	SER	132	15.217	22.587 111.335	1.00 20.93	AAGL
ATOM	1035	CA	SER	132	14.859	23.089 112.654	1.00 19.31	AAGL
ATOM	1036	CB	SER	132	14.444	24.562 112.578	1.00 18.01 1.00 21.72	AAGL AAGL
MOTA	1037	OG	SER	132	13.232	24.709 111.869	1.00 21.72	AAGL
MOTA	1038	С	SER	132 132	13.720 12.766	22.261 113.221 21.930 112.520	1.00 19.32	AAGL
MOTA	1039 1040	Й	ser ile	133	13.842	21.901 114.491	1.00 19.77	AAGL
MOTA MOTA	1040	CA	ILE	133	12.806	21.122 115.143	1.00 20.58	AAGL
MOTA	1042	CB	ILE	133	13.367	20.295 116.317	1.00 21.64	AAGL
ATOM	1043	CG2	! ILE	133	12.297	19.334 116.823	1.00 18.97	AAGL
MOTA	1044		ILE	133	14.644	19.559 115.890	1.00 21.37 1.00 25.39	AAGL AAGL
ATOM	1045		ILE	133	14.515	18.774 114.605	1.00 25.39	AAGL
MOTA	1046	C	ILE ILE	133 133	11.815 11.890	22.142 115.689 22.529 116.850	1.00 21.44	AAGL
MOTA MOTA	1047 1048	о И	GLY	134	10.904	22.581 114.833	1.00 19.14	AAGL
ATOM	1049	CA	GLY	134	9.919	23.560 115.241	1.00 18.88	AAGL
ATOM	1050	С	GLY	134	10.240	24.936 114.690	1.00 18.31	AAGL
ATOM	1051	0	GLY	134	11.344	25.181 114.199		AAGL
ATOM	1052		ASN	135	9.268	25.835 114.769		AAGL
ATOM	1053	CA	ASN	135	9.427	27.201 114.289		AAGL AAGL
ATOM	1054	CB	ASN	135	8.507	27.457 113.097 28.854 112.532		AAGL
ATOM	1055		ASN	135 135	8.666 9.590	29.120 111.759		AAGL
MOTA	1056 1057		l asn 2 asn	135	7.773	29.762 112.932		AAGL
ATOM ATOM	1057		ASN	135	9.044		1.00 17.93	AAGL
ATOM	1059		ASN	135	7.940		1.00 16.64	AAGL
MOTA	1060		GLU		9.967			AAGL

Fig. 3 cont.

MOTA

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## 103/174 30.001 116.865 1.00 17.43 AAGL 9.760 136 MOTA 1061 CA GLU AAGL 1.00 18.10 8.892 31.169 116.371 136 GLU ATOM 1062 CB AAGL 1.00 17.17 9.517 31.970 115.228 1063 CG GLU 136 ATOM 1.00 18.85 AAGL 8.747 33.240 114.867 136 GLU ATOM 1064 CD 33.416 115.314 AAGL 1.00 19.27 7.592 ATOM 1065 OEl GLU 136 1.00 18.05 1.00 17.00 AAGL 34.071 114.120 9.305 136 1066 OE2 GLU MOTA 29.338 118.080 AAGT. .9.116 136 MOTA 1067. С GLU 29.697 118.478 1.00 18.88 AAGL 0 GLU 136 8.013 1068 MOTA AAGL 1.00 16.48 28.379 118.674 9.819 1069 N ILE 137 MOTA 27.657 119.828 1.00 16.33 AAGL 1070 CA ILE 137 9.283 MOTA AAGL 1.00 17.11 9.753 26.185 119.830 137 CB ILE MOTA 1071 25.457 118.615 1.00 18.25 AAGL 9.204 ATOM 1072 CG2 ILE 137 1.00 18.08 AAGL 26.119 119.848 137 11.276 CG1 ILE ATOM 1073 1.00 19.03 AAGL 24.717 120.029 11.822 137 MOTA 1074 CD1 IFE AAGL 1.00 16.65 137 9.600 28.266 121.200 1075 ·ILE MOTA C AAGL 9.770 27.540 122.178 1.00 18.23 1076 137 ATOM 0 ILE AAGL 1.00 15.75 9.668 . 1077 29.591 121.271 ARG 138 N MOTA AAGL 30.265 122.537 . - 9.948 1.00 19.97 MOTA 107B CA ARG 138 31.776 122.327 AAGL 1.00 21.48 138 10.069 1079 CB ARG ATOM 1.00 23.19 AAGL 138 . 10.434 32.559 123.586 ATOM 1080 CG ŖRG 33.946 123.230 1.00 25.82 AAGL 10.971 ARG 138 MOTA 1081 CD 1.00 29.47 AAGL 10.007 34.726 122.454 ME ARG 138 1082 MOTA AAGL 35.263 122.956 1.00 29.69 8.900 1083 CZ ARG 138 ATOM 1.00 32.98 AAGL 35.110 124.243 8.610 1084 NH1 ARG 138 ATOM AAGL 8.075 35.939 122.168 1.00 29.53 138 1085 NH2 ARG MOTA 1.00 20.72 AAGL 29.971 123.557 138 8.852 MOTA 1086 C ARG AAGL 1.00 22.83 29.926 124.755 138 9.112 ARG MOTA 1087 0 29.788 123.081 1.00 19.30 AAGL 7.624 139 1088 N ALA ATOM 1.00 19.27 AAGL 6.513 29.470 123.969 1089 ALA 139. ATOM · CA 1.00 21.29 AAGL 5.268 30.275 123.586 1090 ALA 1,39 MOTA CB 1.00 20.13 AAGL 6.227 27.971 123.893 139 1091 С ALA MOTA 5.102 AAGL 27.517 124.135 1.00 19.76 ATOM 1092 0 ALA 139 27.207 123.565 1.00 16.96 AAGL 140 7.264 1093 N GLY MOTA **NAGL** 1.00 17.78 25.769 123.465 1094 GLY 140 7.124 MOTA CA 25.305 122.102 1.00 18.69 AAGL 6.640 1095 140 ATOM С GLY 1.00 15.87 AAGL 6.669 26.058 121.119 140 1096 0 GLY ATOM 1.00 18.79 AAGL 6.185 24.058 122.051 1097 LEU 141 ATOM N 1.00 18.06 AAGL 23.458 120.815 5,689 LEU 141 MOTA 1098 CA AAGL 6.855 22.900 119.999 1.00 17.19 ATOM 1099 CB LEU 141 AAGL 21.595 120.523 1.00 18,49 1100 CG LEU 141 7.477 MOTA AAGL 1.00 17.04 8.404 21.018 119.457 CD1 LEU 141 ATOM 1101 1.00 17.24 1.00 17.11 AAGL 8.231 21.842 121.827 LEU 141 MOTA 1102 CD2 AAGL 4.741 .22.310 121.145 MOTA 1103 C LEU 141 1.00 19.24 AAGL 21.901 122.295 4.632 0 LEU 141 ATOM 1104 1.00 15.85 AAGL 4.063 21.795 120.126 LEU 142 N MOTA 1105 20.664 120.293 AAGL 3.162 1.00 16.79 MOTA 1106 CA LEU 142 1.00 17.91 AAGL 3.981 19.370 120.301 1107 142 ATOM СВ LEU AAGL 4.783 1.00 18.45 142 19.127 119.017 MOTA 1108 CG LEU AAGL 17.947 119.195 1.00 16.19 5.725 CD1 LEU 142 ATOM 1109 1.00 18.62 AAGL 18.888 117,861 142 3.827 CD2 LEU MOTA 1110 1.00 18.08 AAGL 2.319 20.766 121.562 LEU 142 ATOM 1111 С 1.00 18.47 AAGL 2.374 19.909 122.440 LEU 142 ATOM 1112 O 1.00 18.54 AAGL 21.830 121.652 1.539 TRP 143 ATOM 1113 N 1.00 18.96 AAGL 143 0.684 22.038 122.810 CA TRP MOTA 1114 1.00 17.05 AAGL 0.063 23.431 122.763 ATOM 1115 CB TRP 143 AAGL 1.00 15.57 1.061 24.544 122.780 1116 CG TRP 143 ATOM 1.00 16.04 AAGL 25.920 122.475 0.807 CD2 TRP 143 ATOM 1117 26.621 122.675 AAGL 1.00 15.69 TRP 143 2.014 MOTA 1118 CE2 AAGL -0.324 26.629 122.053 1.00 17.45 CE3 TRP 143 1119 ATOM 24.468 123.139 1.00 15.44 AAGL 2.375 MOTA 1120 CD1 TRP 143 AAGL 1.00 14.73 2.954 25.711 123.081 NE1 TRP 1121 143 ATOM 27.998 122.467 1.00 18.72 AAGL 2.120 MOTA 1122 CZ2 TRP 143 1.00 20.29 AAGL -0.215 28,000 121.848 1123 CZ3 TRP 143 ATOM 1.00 18.09 AAGL 0.995 28.666 122.055 MOTA 1124 CH2 TRP 143 1.00 17.60 AAGL 1125 TRP 143 -0.420 20.989 122.830 ATOM C AAGL 1.00 19.46 -0.860 20.526 121.787 MOTA 1126 O TRP 143 1.00 19.35 AAGL -0.928 20.646 124.022

Fig. 3 cont.

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n m 0 1 4	1120	CD	PRO .	144		19.777 1	24.132	1.00 18.54	AAGL
ATOM ATOM	1128 1129		PRO	144	-0.549	21.167 1	125.340	1.00 18.49	aagl
ATOM	1130		PRO	144	-1.796	20.898 1	126.169	1.00 18.97	AAGL
MOTA	1131	-	PRO	144	-2.228	19.560 1		1.00 20.05	AAGL
ATOM	1132		PRO	144	0.687	20.546		1.00 17.18	AAGL
MOTA	1133	0	PRO	144	1.303	21.162	126.855	1.00 17.80	AAGL
MOTA	1134	·N	LEU	145	1.043	19.329	125.592	1.00 16.38	aagl aagl
ATOM	1135	CA	LEU	145		18.655	126.206	1.00 18.03 1.00 19.70	AAGL
MOTA	1136		LEU	145	2.401	17.277 : 16.208 :	125.50/	1.00 21.47	AAGL
ATOM	1137	CG	LEU	145	1.382 1.529	14.966	125.988	1.00 24.17	AAGL
ATOM	1138	CD1		145 145	1.584	15.871	127.450	1.00 22.76	AAGL
ATOM	1139 . 1140 -		LEO	145	3.482	19.449	126.189	1.00 18.55	AAGL
ATOM ATOM	1140	0	LEU	145	4.291	19.335	127.113	1.00 18.42	AAGL
ATOM	1142		GLY	146	3.671	20.262	125.152	1.00 18.88	AAGL
MOTA	1143	CA	GLY	146	4.884	21.050	125.045	1.00 18.53	AAGL
A'TOM	1144	С	GLY	146	4.759	22.511		1.00 19.09	AAGL '
ATOM	1145	0	GLY	146	5.509		124.948	1.00 17.40	AAGL AAGL
MOTA.	1145	14		147	3.811		126.326	1.00 18.92 1.00 18.48	AAGL
ATOM .		CA	GLU	147	3.647		126.792 127.499	1.00 17.73	AAGL
ATOM	1148	СВ	GLU	147	2.298	24.302	126.565	1.00 18.17	AAGL
MOTA	1149	ÇG	GLU	147	1.111 0.452	25 642	126.328	1.00 21.87	AAGL
MOTA	1150	CD	GLU .	147 147	1.137		126.464	1.00 24.40	AAGL
MOTA MOTA	1151 1152		GLU	147	-0.751		125.997	1.00 22.11	AAGL
MOTA	1153	C	GLU	147	4.789	24.512	127.759	1.00 19.00	AAGL
ATOM	1154	ō	GLU	147	5.421	23.589	128.287	1.00 20.89	AAGL
ATOM	1155	И	THR	148	5.046	25.797	128.003	1.00 18.85	AAGL
ATOM	1156	CA	THR	148	6.137	26.194	128.887	1.00 21.19	AAGL
MOTA	1157	CB	THR	148	6.486		128.746	1.00 21.41 1.00 23.59	. AAGL AAGL
MOTA	1158		THR	148	5.307		128.908	1.00 23.39	AAGL
ATOM	1159		THR	148	7.095		127.379 130.354	1.00 21.10	AAGL
MOTA	1160	C	THR	148	5.889 6.711		131.207	1.00 21.58	AAGL
ATOM	1161	0	thr Ser	148 149	4.753		130.656	1.00 20.92	AAGL
ATOM ATOM	1162 1163	N CA	SER	149	4.487		132.027	1.00 22.49	AAGL
ATOM	1164	CB	SER	149	2.990		132.228	1.00 20.24	AAGL
MOTA	1165	ŌG	SER	149	2.442	23.871	131.142	1.00 21.26	AAGL
ATOM	1166	С	SER	149	5.314		132.275	1.00 23.11	AAGL
MOTA	1167	Ö	SER	149	5.420		133.397	1.00 23.52	AAGL AAGL
MOTA	1168	N	SER	150	5.914		131.205 131.299	1.00 22.32 1.00 22.70	AAGL
MOTA	1169	CA	SER	150	6.749	21.000	131.299	1.00 23.28	AAGL
ATOM	1170	CB	SER-	150	5.925 6:735	10.005	131.058	1.00 24.36	AAGL
MOTA	1171	OG	SER SER	150 150	7.946	21.937	130.345	1.00 22.43	AAGL
MOTA MOTA	1172 1173	C	SER	150	7,909	21.386	129.246	1.00 22.55	AAGL
ATOM	1174	N	TYR	151	9.007	22.619	130.766	1.00 22.50	AAGL
MOTA	1175	CA	TYR	151	10.195		129.932	1.00 23.76	AAGL
ATOM	1176	СВ	TYR	151	11.192	23.730	130.511	1.00 23.66	AAGL
ATOM	1177	CG	TYR	151	10.861	25.169	130.153	1.00 25.07	AAGL
MOTA	1178		TYR	151	10.054		130.978	1.00 22.33 1.00 22.71	aagl aagl
MOTA	1179		LTYR	151	9.719		130.628 128.965	1.00 22.71	AAGL
MOTA	1180		TYR	151	11.329		128.610	1.00 23.11	AAGL
ATOM	1181		TYR	151	10.997 10.195		129.446		AAGL
ATOM	1182		TYR TYR	151 151	9.881		129.116		AAGI
MOTA MOTA	1183 1184	OH	TYR	151	10.827	21.327	129.804	1.00 24.63	AAGL
ATOM	1185		TYR	151	11.627	21.070	128.903	1.00 23.36	AAGL
ATOM	1186		SER	152	10.441		130.703	1.00 25.50	AAGL
ATOM	1187		SER	152	10.942	19.064	130.670	1.00 24.95	AAGL
ATOM	1188		SER	152	10.539		131.945	1.00 25.80	AAGL
ATOM	1189		SER	152	11.051		131.928		AAGL
ATOM	1190	С	SER	152	10.364		129.442		AAGL AAGL
ATOM	1191		SER	152	11.081	17.695	128.696	1.00 24.71 1.00 24.00	AAGL
ATOM	1192		ASN	153	9.059	17 000	2 129.229 5 126.075		AAGL
ATOM	1193			153 153	8.414 6.901	18.108	3 128.073		AAGL
ATOM	1194	СВ	ASN	173	U. 901				

Fig. 3 cont.

					10	31117			
ATOM	1195		ASN	153	6.225	17.239	129.168	1.00 22.68	AAGL
MOTA	1196	OD1		153	6.888	16.579		1.00 21.72 1.00 19.51	aagl aagl
MOTA	1197	ND2		153	4.897	17.235 3 18.486 3		1.00 19.31	AAGL
ATOM	1198		ASN	153	8.970 9.178	17,782	125.702	1.00 19.66	AAGL
ATOM	1199		ASN ILE	153 154	9.192	19.797		1.00 20.58	AAGL
ATOM	1200 1201	N CA	ILE	154	9.733	20.490		1.00 21.12	AAGL
ATOM ATOM	1202	CB	ILE	154	9.922	21.988		1.00 21.27	AAGL
ATOM	1203	CG2		154	10.721	22.626	124.771	1.00 20.30	AAGL .
ATOM	1204	CG1		154	8.563	22.666	126.092	1.00 20.35	AAGL
MOTA	1205	CD1	ILE	154	8.664	24.125		1.00 21.33	AAGL
ATOM	1206	C	ILE	154	11.097	19.901		1.00 22.17	AAGL
ATOM	1207	0	ILE		11.395	19.610		1.00 19.83 1.00 23.65	AAGL AAGL
ATOM	1208	N	GLY	155	11.920 13.246	19.735 19.181		1.00 24.02	AAGL
ATOM	1209 1210	CA C	GLY GLY	155 155	13.240	17.756		1.00 23.51	AAGL
ATOM ATOM	1211	o	GLY	155	13.968	17.384		1.00 23.80	AAGL
MOTA	1212	И	ALA	156	12.300	16.952		1.00 24.34	AAGL
ATOM	1213	CA	ALA	156	12.169	15.560		1.00 23.36	AAGL
MOTA	1214	CB	ALA	156	11.203	14.826		1.00 25.00	AAGL
ATOM	1215	С	AЪA	156	11.701	15.457		1.00 23.25	AAGL
ATOM	1216	0	ALA	156	12.121		123.589	1.00 22.33 1.00 22.39	AAGL AAGL
ATOM	1217	N	LEU	157 157	10.831 10.340		122.538	1.00 22.33	AAGL
MOTA MOTA	1218 1219	CA CB	LEO LEO	157	9.161		122.408	1.00 20.00	AAGL
ATOM	1220	CG	LEU	157	7.868		123.059	1.00 22.93	AAGL
ATOM	1221		LEU	157	6.894	17.994	123.274	1.00 22.57	AAGL
ATOM	1222	CD2	LEU	157	7.260		122.164	1.00 21.07	AAGL
MOTA	1223	С	<i>LEU</i>	157	11.443		121.564	1.00 21.89	AAGL
ATOM	1224	0	LEU	157	11.616		120.518	1.00 20.81 1.00 21.14	aagl aagl
ATOM	1225	N	LEU	158 158	12.195 13.267		121.021	1.00 21.14	AAGL
MOTA MOTA	1226 1227	CA CB	LEU	158	13.903		121.569	1.00 22.22	AAGL
ATOM	1228	CG	LEU	158	12.982		121.562	1.00 21.62	AAGL
ATOM	1229		LEU	158	13.640	21.917	122.316	1.00 21.34	AAGL
ATOM	1230	CD2	LEU	158	12.683		120.131	1.00 21.57	AAGL
MOTA	1231	C	LEU	158	14.299		120.880	1.00 24.78	aagl aagl
MOTA	1232	0	LEU	158	14.807 14.584		119.794 121.990	1.00 23.68 1.00 24.81	AAGL
MOTA MOTA	1233 1234	N CA	HIS HIS	159 159	15.518		122.009	1.00 26.46	AAGL
ATOM	1235	CB	HIS	159	15.566		123.423	1.00 27.84	AAGL
ATOM	1236	CG	HIS	159	16.473	13.553	123.563	1.00 30.73	AAGL
ATOM	1237	CD2	HIS	159	16.204		123.812	1.00 32.59	AAGL
ATOM	1238	ND1	HIS	159	17.845		123.482	1.00 31.02	AAGL
MOTA	1239		HIS	159	18.383		123.676	1.00 32.44	AAGL AAGL
ATOM	1240		HIS	159	17.409		123.880 121.017	1.00 33.23 1.00 26.31	AAGL
MOTA MOTA	1241 1242	С 0	HIS HIS	159 159	15.029 15.796		120,190	1.00 26.14	AAGL
MOTA	1243	и	SER	160	13.749		121.110	1.00 25.57	AAGL
ATOM	1244	CA	SER	160	13.149	12.927	120.220	1.00 26.09	AAGL
ATOM	1245	CB	SER	160	11.679		120.590	1.00 26.91	AAGL
MOTA	1246	OG	SER	160	11.555		121.857	1.00 28.98	AAGL
MOTA	1247	С	SER	160	13.225		118.745		aagl aagl
ATOM	1248	0	SER	160	13.564		117.885 118.452	1.00 26.49 1.00 22.94	AAGL
MOTA	1249	N CA	GLY GLY	161 161	12.890 12.934		117.078	1.00 22.94	AAGL
MOTA MOTA	1250 1251	CA	GLY	161	14.359		116.556		AAGL
MOTA	1252	ō	GLY	161	14.631		115.450		AAGL
ATOM	1253	Ŋ	ALA		15.277	15.519	117.368	1.00 24.30	AAGL
MOTA	1254	ÇA	ALA	162	16.683		117.002		AAGL
MOTA	1255	CB	ALA		17.510		118.164		AAGL
ATOM	1256		ALA		17.172		116.598		AAGL AAGL
ATOM	1257	0	ALA		17.801 16.876		115.546 117.423		AAGL
ATOM	1258 1259	n Ça	TRP TRP		17.320		117.124		AAGL
MOTA MOTA	1259		TRP		17.222		118.368		AAGL
MOTA	1261	CG	TRP		18.386		119.245		AAGL

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ATOM	1262	CD2	TRP	163	19.668	10.565 119.134	1.00 32.43	AAGL
ATOM	1263		TRP	1.63	20.516	11.194 120.068	1.00 31.66	AAGL
MOTA	1264	CE3	TRP	163	20.185	9.541 118.329	1.00 32.40	AAGL
MOTA	1265	CD1	TRP.	163 .	18.497	12.130 120.217	1.00 31.49 1.00 32.86	AAGL AAGL .
MOTA	1266	NE1		163		12.149 120.715	1.00 32.68	AAGL .
ATOM	1267	CZ2		163 .		10.836 120.223 9.184 118.479	1.00 32.50	AAGL
MOTA	1268	CZ3		163	21.522	9.832 119.421	1.00 32.64	AAGL
MOTA	1269	CH2		163	22.342	11,144 115.952	1.00 27.25	AAGL
ATOM	1270	C	TRP	163 163	16.636 17.177	10.205 115.372	1.00 28.73	AAGL
ATOM	1271	0	TRP	164	15.448	11.613 115.598	1.00 25.57	AAGL
MOTA	1272 1273	N CA	<b>GLY</b>	164	14.782	11.045 114.445	1.00 24.90	AAGL
ATOM ATOM	1274	C	GLY	164	15.651	11.409 113.253	1.00 26.22	AAGL
ATOM	1275	ō	GLY	164	15.831	10.618 112.326	1.00 26.72	AAGL
MOTA	1276	N	VAL	165	16.206 [.]	12.618 113.290	1.00 25.62	. AAGL ,
MOTA	1277	CA	VAL	165	17.078	13.087 112.219	1.00 26.48	AAGL
ÁTOM	1278	CB	VAL	165	17.379	14.598 112.356	1.00 26.61	· · AAGL AAGL
MOTA	1279		VAL	165	18.398	15.026 111.293	1.00 23.67 1.00 25.11	AAGL
MOTA	1280		VAL	165		15.397 112.216 12.328 112.251	1.00 23.11	AAGL
ATOM	1281	С	VAL	165	18.406	11.788 111.233	1.00 29.75	AAGL
MOTA	1282	0	VAL .	165	18.850 19.037	12.295 113.420	1.00 27.66	AAGL
MOTA	1283	N	LYS	166 166	20.313	11.607 113.581	1.00 29.81	AAGL
MOTA	1284 1285	CA CB	LYS LYS	166	20.770	11.661 115.045	1.00 29.36	AAGL.
MOTA MOTA	1286	CG	LYS	166	21.062	13.060 115.590	1.00 30.72	AAGL
ATOM	1287	CD	LYS	166	21.442	12.982 117.065	1.00 33.25	AAGL
MOTA	1288	CE	LYS	166	21.674	14.358 117.677	1.00 33.72	AAGL
ATOM	1289	NZ	LYS	166	22.883	15.036 117.122	1.00 33.70	AAGL
MOTA	1290	С	LYS	166	20.229	10.144 113.136	1.00 31.30	AAGL
ATOM	1291	0	LYS	166	21.206	9.594 112.622	1.00 31.56	aagl aagl
· ATOM	1292	N	ASP	167	19.065	9.519 113.319	1.00 30.83 1.00 32.56	AAGL .
MOTA	1293	CA	ASP	167	18.893	8.116 112.944 7.442 113.854	1.00 32.30	AAGL
ATOM	1294	CB	ASP	167	17.863	7.187 115.245	1.00 33.01	AAGL
MOTA	1295	CG	ASP	167 167	18.387 19.620	7,148 115.425	1,00 33.60	AAGL
ATOM	1296		ASP	167	17.558	7.006 116.160	1.00 32.14	AAGL
MOTA MOTA	1297 1298	C		· 167	18.481	7.858 111.494	1.00 33.63	AAGL
ATOM	1299	ö	ASP	167	18.347	6.696 111.082	1.00 32.89	AAGL
ATOM	1300	N	SER	168	18.280	8.925 110.724	1:00 31.74	AAGL
MOTA	1301	CA	SER	168	17.846	8.786 109.341	1.00 31.90	AAGL
ATOM	1302	CB	SER	168	17.279	10.111 108.823	1.00 29.91	aagl aagl
MOTA	1303	QG	SER	168	18.301	11.074 108.654	1.00 30.10 1.00 32.86	AAGL
ATOM	1304	С	SER	168	18.922	8.294 108.378	1.00 32.80	AAGL
ATOM	1305	0	SER	168	20.114	8.248 108.704 7.950 107.179		AAGL
MOTA	1306	N	ASN	169	18.470 19.328	7.430 106.123		AAGL
ATOM	1307	ÇA	ASN ASN	169 169	18.493	6.545 105.195		AAGL
ATOM	1308 1309	CB CG		169	17.848	5.377 105.925		AAGL
ATOM ATOM	1310		L ASN	169	16.833	4.841 105.482		AAGL
ATOM	1311		2 ASN	169	18.440	4.971 107.044	1.00 39.67	AAGL
ATOM	1312		ASN	169	20.043	8.508 105.308		AAGL
ATOM	1313		ASN	169	20.725	8.194 104.324	1.00 39.86	AAGL
ATOM	1314	N	LEU	170	19.891	9.773 105.695		AAGL
ATOM	1315			170	20.562	10.849 104.966	1.00 39.07	aagl aagl
MOTA	1316			170	20.133	12.222 105.502		AAGL
ATOM	1317			170	18.784	12.783 105.053 14.122 105.733		AAGL
MOTA	1318		1 LEU	170	18.533	12.960 103.548		AAGL
ATOM	1319		2 LEU	170	18.775 22.068	10.672 105.146		AAGL
ATOM	1320		LEU	170 170	22.580	10.787 106.257		AAGL
MOTA	1321 1322		ALA	171	22.770	10.392 104.050		AAGL
MOTA MOTA	1322			171	24.219	10.180 104.078	3 1.00 44.92	AAGL
ATOM	1323				24.796		1.00 45.32	AAGL
ATOM	1329		ALA		24.913	11.063 105.117	7 1.00 45.99	AAGL
ATOM	1326		ALA		25.671	10.568 105.962	2 1.00 47.05	AAGL
ATOM	1327		THR		24.668	12.370 105.044		AAGL
ATOM	1328				25.246	13.316 105.998	3 1.00 45.78	AAGL

Fig. 3 cont.

					10			
ATOM	1329		THR	172	25.856	14.549 105.320	1.00 46.89	aagl aagl
MOTA	1330	OG1		172	26.551	14.167 104.132	1.00 48.14	AAGL
ATOM	1331		THR	172	26.822	15.224 106.269	1.00 46.74 1.00 44.10	AAGL
ATOM	1332		THR	172	24.117	13.844 106.868	1.00 44.10	AAGL
MOTA	1333		THR	172	23.086	14.272 106.351 13.835 108.179	1.00 44.90	AAGL
ATOM	1334		CHR.	173	24.311	14.319 109.088	1.00 39.37	AAGL
MOTA	1335		THR	173	23.283 23.621	13.926 110.530	1.00 39.69	AAGL
MOTA	1336		THR	173 173	23.691	12.497 110.620	1.00 40.97	AAGL
MOTA	1337 1338	OG1 'CG2 '	THR	173	22.555	14.436 111.494	1.00 40.31	AAGL
ATOM ATOM	1339		THR	173	23.140	15.837 108.969	1.00 36.34	AAGL
MOTA	1340		THR	173	24.118	16.581 109.083	1.00 35.72	AAGL
ATOM	1341		PRO	174	21.916	16.319 108.702	1.00 33.51	AAGL
ATOM	1342		PRO	174	20.709	15.592 108.274	1.00 33.11	AAGL
ATOM	1343	CA	PRO	174	21.728	17.766 108.580	1.00 30.76	AAGL
MOTA	1344	CB	PRO	174	20.252	17.891 108.223	1.00 31.41	AAGL
ATOM	1345	CG (	PRO	174	19.989	16.624 107.452	1.00 33.06	AAGL
MOTA	1346	С	PRO	174	22.056	18.475 109.883	1.00 27.61	AAGL
ATOM	1347		PRO	174	22.074	17.865 110.945	1.00 26.79	AAGL AAGL
MOTA	1348		LYS	175	22.332	19.767 109.800	1.00 28.61 1.00 27.46	AAGL
MOTA	1349		LYS	175	22.614	20.541 111.001 21.917 110.636	1.00 27.40	AAGL
ATOM	1350		LYS	175	23.167 24.679	22.002 110.611	1.00 35.14	AAGL
MOTA	1351		LYS	175 175	25.286	20.926 109.751	1.00 39.94	AAGL
ATOM ·	1352 1353		LYS LYS	175	26.804	21.046 109.733	1.00.42.54	AAGL
ATOM ATOM	1354		LYS	175	27.396	20.867 111.091	1.00 43.56	AAGL
ATOM	1355		LYS	175	21.267	20.693 111.695	1.00 26.21	AAGL
MOTA	1356		LYS	175	20.297	21.096 111.068		AAGL
ATOM	1357	N	ILE	176	21.209	20.350 112.975		AAGL
MOTA	1358	CA	ILE	176	19.968	20.443 113.728		AAGL
ATOM	1359	CB	ILE	176	19.899	19.320 114.779		AAGL
ATOM	1360	CG2	ILE.	176	18.689	19.515 115.676		AAGL
MOTA	1361	CG1	ILE	176	19.847	17.964 114.061		AAGL
ATOM	1362	CD1		176	20.148	16.775 114.941		AAGL AAGL
MOTA	1363	С	ILE	176	19.866	21.807 114.395		AAGL
MOTA	1364	0	ILE	176	20.752	22.208 115.136 22.507 114.127		AAGL
MOTA	1365	0T	MET	177 177	18.769 18.557	23.847 114.656		AAGL
MOTA	1366 1367	CA CB	MET MET	177	18.401	24.837 113.488	the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the s	. AAGL
MOTA MOTA	1368	CG	MET	177	17.934	26.249 113.903		AAGL
ATOM	1369	SD	MET	177	17.586	27.336 112.488		AAGL
MOTA	1370	CE	MET	177	19.288	27,706 111.969	1.00 22.76	AAGL
ATOM	1371	c	MET	177	17.352	24.013 115.576		AAGL
ATOM	1372	0	MET	177	16.343	23.326 115.425		AAGL
ATOM	1373	N	ILE	178	17.485	24.927 116.534		AAGL
ATOM	1374	CA	ILE	178	16.395	25.294 117.433		AAGL
MOTA	1375	CB	ILE	178	16.750	25.134 118.932		AAGL
ATOM	1376		ILE	178	15.678	25.810 119.798		AAGL AAGL
MOTA	1377		ILE	178	16.830	23.647 119.28	1.00 23.39 7 1.00 25.76	AAGL
ATOM	1378		ILE	178	17.014	23.363 120.76		AAGL
ATOM	1379	Č	ILE	178	16.204	26.766 117.088 27.555 117.12		AAGL
MOTA	1380	0	ILE	178	17.156 14.971	27.125 116.75		AAGL
MOTA	1381	N	HIS	179 179	14.632	28.475 116.31		AAGL
MOTA	1382 1383	CA CB	HIS	179	14.054	28.356 114.89		AAGL
Mota Mota	1384	CG	HIS	179	13.454	29.617 114.36		AAGL
ATOM	1385		HIS	179	13.731	30.919 114.60		AAGL
ATOM	1386		HIS		12.438	29.611 113.43		aagl
ATOM	1387		HIS		12.114	30.855 113.12	9 1.00 16.27	AAGL
ATOM	1388		HIS	179	12.883	31.668 113.83	0 1.00 17.92	AAGL
ATOM	1389	С	HIS		13.658	29.235 117.22	7 1.00 20.10	AAGL
ATOM	1390	ō	HIS		12.541	28.780 117.47		AAGL
MOTA	1391	И	LEU		14.090	30.394 117.71		AAGI
ATOM	1392		LEU		13.258	31.237 118.57		AAGL
MOTA	1393	CB	FEO		13.930	31.480 119.92		AAGI AAGI
ATOM	1394	CG	LEU		14.253	30.306 120.85	4 1.00 24.61	
MOTA	1395	CD1	LEU	180	14.701	30.866 122.20	8 1.00 23.57	AAGI

1462

## 108/174 1.00 22.59 AAGL 29.405 121.029 13.038 180 CD2 LEU ATOM 1396 32.588 117.905 1.00 20.35 AAGL 13.027 1397 C LEU 180 ATOM 1.00 20.34 AAGL 33.032 117.099 180 13.838 LEU MOTA 1398 ٥ 33.237 118.240 1.00 19.30 AAGL 11.918 181 ATOM 1399 N ASP 34.548 117.688 AAGL 1.00 19.90 181 11.623 ASP 1400 CA ATOM AAGL 34.796 117.680 1.00 21.15 10.112 181 1401 ASP MOTA CB 34.825 119.070 AAGL 1.00 22.95 1402 ASP 181 9.522 CG MOTA AAGL 9.910 33.973 119.900 1.00 22.67 181 1403 0D1 ASP ATOM 35.697 119.336 AAGL 1.00 25.18 1404 181 8.664 OD2 ASP MOTA AAGL 1.00 21.86 12.315 35.580 118.576 181 ATOM 1405 С ASP 35.218 119.524 1.00 23.76 AAGL 181 13.020 1406 O ASP ATOM AAGL 182 12.107 36.856 118.271 1.00 22.19 1407 N ASP MOTA 37.948 119.034 1.00 22.68 AAGL 182 . 12.718 MOTA 1408 CA ASP AAGL .38.129 120.381 - 1.00 24.73 182 12.013 MOTA 1409 СВ ASP 38.605 120.234 1.00 26.20 AAGL 182 .10.589 1410 CG ASP ATOM . AAGL 1.00 30.46 10.226 39.052 119.134 182 ATOM 1411 OD1 ASP 38.539 121.226 1.00 30.54 AAGL 9.829 OD2 ASP 182 ATOM 1412 1.00 21.94 AAGL 182 14.205 37.719 119.282 1413 ASP ATOM С 37.656 120.432 1.00 22.68 AAGL 14.645 1414 ASP 182 ATOM O 1.00 21.90 AAGL 37.610 118.203 183 · 14.975 GLY ATOM 1415 N AAGL 1.00 20.97 37.388 118.334 183 16.403 1416 CA GLYMOTA AAGL 38.524 119.003 1.00 21.01 183 17.158 ATOM 1417 С GLY AAGL 38.340 119.478 1.00 24.20 18.279 183 1418 GLY ATOM 0 AAGL 39.701 119.045 1.00 23.43 TRP 184 16.550· 1419 N MOTA 1.00 25.63 AAGL 40.859 119.655 184. 17.191 ATOM 1420 CA TRP 1.00 24.89 AAGL 16.514 42.141 119.173 184 1421 CB TRP MOTA 1.00 27.09 AAGL 15.045 42.120 119.376 184 MOTA 1422 CG TRP 1.00 28.81 AAGL 42.467 120.576 14.346 TRP 184 MOTA 1423 CD2 1.00 28.20 AAGL 12.971 42.248 120.336 184 TRP MOTA 1424 CE2 14.750 1.00 30.34 AAGL 42.944 121.833 1425 CE3 TRP 184 ATOM AAGL 1.00 27.72 41.717 118.481 14.098 CD1 TRP 184 ATOM 1426 41.792 119.049 AAGL 1.00 27.27 12.847 1427 NE1 TRP 184 ATOM . AAGL 1.00 32.25 42.487 121.308 184 11,994 1428 CZ2 TRP ATOM 1.00 33.25 AAGL 13.776 43.184 122.802 184 ATOM 1429 CZ3 TRP 42.954 122.533 1.00 30.56 AAGL 184 12.414 1430 CH2 TRP MOTA AAGL 1.00 27.12 184 17.155 40.816 121.184 TRP MOTA 1431 С 1.00 26.68 AAGL 41.563 121.850 17.869 TRP 184 ATOM 1432 0 1.00 26.77 AAGL 16.332 39.935 121.742 185 SER ATOM 1433 N AAGL 16.207 1.00 28.56 39.846 123.190 MOTA 1434 CA SER 185 1.00 28.06 AAGL 14.739 39.648 123.558 185 1435 CB SER ATOM AAGL 39.465 124.949 1.00 31.97 14.594 185 MOTA 1436 OG SER 1.00 27.96 AAGL 38.761 123.858 17.055 SER 185 MOTA 1437 C 37.600 123.919 1.00 29.29 AAGI. 16.660 185 ATOM 1438 0 SER 39.142 124.374 AAGL 1.00 27.87 18.218 1439 N TRP 186 MOTA 1.00 27.87 AAGL 19,091 38.176 125.032 186 MOTA 1440 CA TRP 20.380 38.853 125.511 1.00 29.10 AAGL ATOM 1441 CB TRP 186 1.00 27.39 AAGL 186 21.165 38.036 126.509 1442 TRP ATOM CG 1.00 29.36 AAGL 21.670 36.705 126.335 MOTA 1443 CD2 TRP 186 1.00 30.06 AAGL 36.352 127.531 CE2 TRP 186 22.338 MOTA 1444 1.00 30.04 AAGL 21.625 35.774 125.285 1445 CE3 TRP 186 ATOM 1.00 29.3B AAGL 38,422 127.765 CD1 TRP 186 21.534 1446 MOTA 22.239 37.417 128.386 1.00 28.39 AAGL 186 1447 NE1 TRP ATOM 1.00 30.53 AAGL 35.108 127.705 1448 CZ2 TRP 186 22.957 MOTA AAGL 22.240 34.540 125.459 1.00 30.87 186 ATOM 1449 CZ3 TRP 1.00 31.05 AAGL 34.218 126.662 22.898 186 1450 CH2 TRP ATOM AAGL 1.00 28.13 186 18.418 37.486 126.217 TRP MOTA 1451 C 1.00 27.04 AAGL 36.291 126.445 18,620 TRP 186 MOTA 1452 Q 1.00 28.09 AAGL 17.628 38.232 126.979 187 1453 ASP ATOM N 1.00 29.42 37.643 128.131 AAGL 16.961 1454 ASP 187 ATOM CA AAGL 1.00 32.15 16.156 38.704 128.887 ASP 187 1455 CB MOTA 17.028 39.817 129.450 1.00 37.52 AAGL ASP 187 MOTA 1456 CG AAGL 1.00 39.29 18.255 39.612 129.611 1457 OD1 ASP 187 ATOM AAGL 40.896 129.748 1.00 41.44 16.476 ASP 187 MOTA 1458 OD2 1.00 28.91 AAGL 16.035 36.488 127.724 187 1459 ASP MOTA С AAGL 1.00 27.77 16.033 35.431 128.357 1460 ASP 187 ATOM 0 1.00 27.43 AAGL 36.691 126.668 15.250 GLN 188 ATOM 1461 N AAGL 35.657 126.215 1.00 27.67 188 14.326 ATOM CA GLN

Fig. 3 cont.

## 109/174 36.220 125.170 AAGL 1.00 28.11 13.357 GLN 188 CB ATOM 1463 37.066 125.735 AAGL 1.00 31.74 188 12.222 MOTA 1464 CG GLN 36.258 126.588 1.00 36.22 AAGL 11.247 188 GLN MOTA 1465 CD AAGL 35.103 126.274 10.921 1.00 36.68 188 1466 OE1 GLN MOTA 1.00 37.18 AAGL 36.867 127.660 . 188 10.760 ATOM 1467 NE2 GLN 34.456 125.641 1.00 26.39 AAGL 15.061 188 GLN ATOM 1468 C AAGL 33.318 125.934 1.00 26.19 14.710 188 GLN ATOM 1469 0 34.712 124.829 AAGL 1.00 25.52 16.086 189 ATOM 1470 N GLN 1:00 24.65 AAGL 33.633 124.225 16.864 189 **GLN** MOTA 1471 CA 34.191 123.351 1.00 24.63 AAGL 17.997 189 1472 CB GLN ATOM 1.00 24.46 AAGL 17.576 34.991 122.126 189 MOTA 1473 CG GLN AAGL 34.191 121.149 1.00 21.93 16.736 1474 189 ATOM CD GLN 1.00 20.15 33.084 120.760 AAGL 17.097 189 1475 OE1 GLN MOTA 34.759 120.739 1.00 23.53 AAGL 1476 GLN 189 15.613 MOTA NE2 AAGL 1.00 25.42 1477 17.484 32.759 125.308 GLN 189 С ATOM 31.544 125.324 1.00 23.58 AAGL 17.314 1478 GLN 189 MOTA 0 1.00 25.59 AAGL 33.405 126.219 1479 190 18.199 ASN N ATOM 32.725 127.293 AAGL 1.00 26.28 18.892 1480 ASN 190 ATOM CA 1.00 28.08 AAGL 19.745 33.736 128.056 190 1481 ASN CB ATOM AAGL 1.00 29.88 33.091 129.135 20.593 ATOM 1482 CG ASN 190 1.00 29.87 AAGI 190 21.204 32.041 128.922 1483 OD1 ASN ATOM 33.727 130.295 1.00 33.02 AAGL 20.649 190 ATOM 1484 ND2 ASN AAGL 31.970 128.250 1.00 26.80 1485 ASN 190 17.978 C ATOM AAGL 1.00 27.29 30.866 128.675 18.300 190 ATOM 1486 0 ASN 32.554 128.590 1.00.27.59 AAGL 1487 N TYR 191 16.838 ATOM 1.00 27.82 AAGL 31.878 129.504 191 15.931 MOTA 1488 CA TYR 32.767 129.832 1.00 28.23 AAGL 14.735 ATOM 1489 CB TYR 191 1.00 30.08 AAGL 13.815 32.132 130.844 191 TYR MOTA 1490 CG 31.294 130.446 1.00 32.24 AAGL 12.775 CD1 TYR 191 ATOM 1491 AAGL 1.00 33.28 CE1 TYR 191 11.975 30.641 131.385 ATOM 1,492 32.308 132.210 1.00 31.47 AAGL 14.032 1493 TYR 191 ATOM CD2 AAGL 1.00 31.82 191 13.240 31.662 133.157 TYR MOTA 1494 CE2 30.830 132.739 1.00 34.47 AAGL 12.219 1495 191 ATOM CZ TYR 1.00 36.38 AAGL 11.458 30.168 133.679 TYR 191 1496 OH MOTA AAGL 15.443 30.551 128.929 1.00 27.27 191 MOTA 1497 C TYR 1.00 25.68 AAGL 15.392 29.537 129.631 1498 TYR 191 ATOM 0 1.00 25.48 AAGL 15.079 30.557 127.651 1499 PHE 192 ATOM N AAGL 1,00 26.24 1500 CA PHE 192 14.605 29.341 127.016 MOTA AAGL 29.593 125.541 1.00 24.60 14.260 MOTA 1501 Ç₿ PHE 192 1.00 22.89 AAGL 28.351 124.799 192 13.854 1502 CG PHE MOTA AAGL 27.893 124.848 1.00 23.14 CD1 PHE 192 12.541 ATOM 1503 27.607 124.098 AAGL 1.00 22.70 14.795 192 1504 CD2 PHE MOTA 1.00 22.64 AAGL 26.706 124.208 12.169 192 ATOM 1505 CE1 PHE AAGL 26,417 123,455 1.00 22.68 14.439 1506 CE2 PHE 192 ATOM AAGL 1.00 23.16 25.965 123.510 13.125 PHE 192 MOTA 1507 CZ 28.237 127.095 1.00 26.50 AAGL 192 15.651 ATOM 1508 С PHE 1.00 25.06 AAGL 27,154 127,612 192 15.386 ATOM 1509 0 PHE 1.00 26.97 AAGL 28.513 126.577 16.847 TYR 193 MOTA 1510 N 1.00 28.47 AAGL 17.898 27.510 126.570 193 MOTA 1511 CA TYR 1.00 25.93 AAGL 27.991 125.704 TYR 193 19.066 MOTA 1512 CB AAGL 1.00 26.36 18.675 28.113 124.243 193 1513 TYR MOTA CG 1.00 24.37 AAGL 26.979 123.498 18.344 1514 CD1 TYR 193 MOTA 1.00 23.29 AAGL 193 17.905 27.084 122.178 TYR MOTA 1515 CE.1 AAGL 18.561 29.357 123.632 1.00 26.34 1516 CD2 TYR 193 MOTA 1.00 24.57 AAGL 18.121 29.474 122.307 TYR 193 1517 CE2 MOTA AAGL 1.00 23.44 17.797 28.331 121.592 MOTA 1518 CZ TYR 193 1.00 24.47 AAGL 17.370 28.431 120.290 ATOM 193 1519 OH TYR 27.087 127.952 1.00 28.72 **AAGL** 18.384 MOTA 1520 С TYR. 193 1.00 29.46 AAGL 193 18.542 25.892 128.212 0 TYR 1521 MOTA 28.046 128.844 1.00 30.56 AAGL 18.610 MOTA 1522 N GLU 194 1.00 32.74 AAGL 194 19.081 27.684 130.177 CA GLU 1523 MOTA 28.921 131.048 1.00 36.66 AAGL 19.344 1524 СВ GLU 194 MOTA 1.00 42.88 AAGL 194 20.119 28.543 132.325 1525 CG GLU MOTA AAGL 29.668 133.327 1.00 46.55 20.271 1526 CD GŁU 194 MOTA AAGL 1.00 48.27 21.086 29,502 134.275 1527 OE1 GLU 194 MOTA AAGL 1.00 47.67 19.580 30.704 133.194 1528 OE₂ GLU 194 MOTA

Fig. 3 cont.

18.056

1529

ATOM

C

GLU

194

26.802 130.875

1.00 31.54

AAGL

110/174 AAGL 25.764 131.445 1.00 31.58 18.396 194 1530 0 GLU ATOM AAGL 1.00 30.56 27.212 130.823 16.795 THR 195 N 1531 MOTA AAGL 26.453 131.468 1.00 28.40 195 15.731 THR 1532 CA ATOM 1.00 27.94 AAGL 27,226 131.402 14.408 1533 CB THR 195 ATOM AAGL 28.545 131.929 1.00 25.50 195 14.611 THR 1534 0G1 MOTA AAGL 1.00 26.24 26.516 132.211 13.330 195 THR 1535 CG2 ATOM 1.00 28.06 AAGL 25.054 130.868 195 15.535 THR MOTA 1536 С AAGL 1.00 26.71 24.071 131.599 15,427 195 THR ATOM 1537 1.00 27.08 AAGL 24.961 129.545 15.486 196 N VAL 1538 ATOM AAGL 23.666 128.902 1.00 27.16 196 15.301 ATOM 1539 CA VAL 1.00 29.10 **AAGL** 23.838 127.369 15.035 196 CB VAL 1540 MOTA AAGL 24.510 126.700 1.00 30.65 196 16.227 VAL 1541 CG1 ATOM .1.00 31.18 AAGL 14.748 22.487 126.727 196 1542 CG2 VAL ATOM AAGL 22.736 129.137 1.00 26.59 16.502 196 1543 С VAL ATOM AAGL 1.00 25.06 16.330 21.563 129.449 196 1544 0 VAL ATOM AAGL 23.266 129.015 1.00 26.11 17.716 LEU 197 1545 И MOTA AAGL 1.00 28.97 10.911 22.451 129.214 LEU 197 1546 CA ATOM AAGL 23.207 128.735 1.00 29.84 1.97 20.161 LEU MOTA 1547 CB 1.00 30.49 AAGL -23.474 127.220 20.233 1,97 LEU ATOM 1549 CG AAGL 24.445 126.927 1.00 32.56 21.377 197 LEU CD1 ATOM 1549 AAGL 1.00 30.05 22.176 126.464 20.413 197 1550 CD2 LEU ATOM 1.00 28.89 AAGL 19.069 22.032 130.674 197 LEU MOTA 1551 С AAGL 20.976 130.971 1.00 30.68 19.632 197 LEU 1552 0 ATOM 1.00 29.81 AAGL 22.844 131.586 18.550 1553 N ALA 198 ATOM AAGL 22.530 133.008 1.00 30.14 18.646 198 CA ALA MOTA 1554 1.00 29.46 AAGL 18.110 23.688 133.831 198 ALA 1555 CB MOTA AAGL 21.237 133.387 1.00 31.06 17.913 198 ALA ATOM 1556 C 1.00 30.62 AAGL 20.624 134.411 18.223 198 0 ALA MOTA 1557 AAGL 20.814 132.569 1.00 30.12 16.951 199 THR MOTA 1558 М AAGL 1.00 29.04 19.599 132.868 16.192 199 1559 CA THR ATOM AAGL 19.569 132.137 1.00 30.14 14.831 199 1560 CB THR MOTA AAGL 19.375 130.735 1.00 28.92 199 15.051 THR ATOM 1561 OG1 1.00 28.52 AAGL 20.876 132.351 14.058 199 THR ATOM 1562 CG2 AAGL 18.306 132.497 1.00 30.21 16.926 199 THR ATOM 1563 C AAGL 1.00 31.94 17.237 133.006 16.602 1564 THR 199 ATOM 0 AAGL 1.00 29.95 17.907 18.406 131.613 200 GLY 1565 N MOTA AAGL 17.219 131.194 1.00 30.95 200 18.626 1566 CA GLY MOTA AAGL 16.428 130.143 1.00 31.30 200 17.868 С GLY 1567 ATOM 1.00 31.90 AAGL 15.436 129.625 18.376 200 MOTA 1568 О GLY AAGL 1.00 31.18 16.647 16.850 129.823 201 1569 N GLU ATOM AAGL 16.145 128.813 1.00 30.31 201 15.856 GLU 1570 CA ATOM 1.00 29.74 AAGL 16.557 128.881 14.385 1571 GLU 201 ATOM CB AAGL 1.00 32.87 16.062 130.110 201 13.640 GLU 1572 CG MOTA 1.00 33.76 AAGL 14.555 130.285 13.710 201 MOTA 1573 CD GLU AAGL 13.833 129.274 1.00 34.18 13.838 201 1574 OE1 GLU MOTA AAGL 14.086 131.443 1.00 34.63 13.617 OE2 GLU 201 MOTA 1575 1.00 28.94 AAGL 16.399 16.440 127.423 1576 С GLU 201 ATOM AAGL 15.625 126.511 1.00 27.79 16.271 201 GLU 1577 MOTA 0 1.00 28.10 AAGL 16.988 17.623 127.272 MOTA 1578 N LEU 202 18.033 126.009 AAGL 1.00 28.10 202 17.587 LEU 1579 CA ATOM 1.00 28.75 AAGL 19.376 125.548 17.029 202 MOTA 1580 CB LEU AAGL 1.00 27.26 19.987 124.350 LEU 202 17.766 CG 1581 ATOM AAGL 1.00 27.62 17.461 19.196 123.090 202 ATOM 1582 CD1 LEU AAGL 21.430 124.178 1.00 29.02 17.337 CD2 LEU 202 1583 ATOM AAGL 1.00 28.79 19.088 18.170 126.240 202 LEU 1584 С ATOM AAGL 18.888 127.141 1.00 29.33 19.518 ATOM 1585 0 LEU 202 AAGL 1.00 29.74 17.473 125.433 203 19.875 LEU MOTA 1586 N AAGL 1.00 32.35 17.524 125.557 21.326 203 LEU ATOM 1587 CA 16.146 125.271 1.00 33.32 AAGL LEU 203 21.920 MOTA 1588 CB 1.00 33.68 AAGL 21,643 15.084 126.328 203 CG **PEA** MOTA 1589 AAGL 13.828 125.998 1.00 38.12 22.436 CD1 LEU 203 1590 ATOM 1.00 37.93 AAGL 22.053 15.615 127.694 203 CD2 LEU ATOM 1591 AAGL 18.541 124.603 1.00 32.26 21.934 LEU 203 1592 C MOTA AAGL 1.00 33.19 18.694 123.474 21,475 203 1593 O LEU ATOM AAGL 19.231 125.055 1.00 33.40 22.975 204 1594 N SER MOTA 1.00 34.27 AAGL 20.215 124.213 204 23.634 1595 CA SER ATOM AAGL 1.00 34.70 24.824 20.826 124.947 204 1596 CB SER ATOM

Fig. 3 cont.

111/174 1.00 36.69 AAGL 21.894 124.194 25.380 204 1597 SER ATOM OG 19.529 122.934 1.00 34.03 AAGL 204 24.103 SER 1598 C MOTA AAGL 1.00 35.28 24.163 20.145 121.871 SER 204 ATOM 1599 0 18.248 123.043 1.00 32.63 AAGL THR 205 24.438 ATOM 1600 N AAGL 1.00 33.11 24.890 17.491 121.880 205 THR MOTA 1601 CA 16.204 122.302 1.00 33.97 AAGL 25.650 THR 205 CB MOTA 1602 1.00 35.21 AAGL 24.875 15,458 123.256 THR 205 1603 OG1 ATOM 16.572 122.919 1.00 34.51 AAGL 26.989 THR 205 ATOM 1604 CG2 1.00 32.07 AAGL 17.111 120.951 23.737 205 THR 1605 С · ATOM 16.584 119.865 1.00 32.54 AAGL 23.960 205 1606 O THE MOTA AAGL 1.00 30.83 17.389 121.367 22.504 ASP 206 MOTA 1607 N 17.054 120.536 1.00 29.51 AAGL 21.352 ASP 20€ 1608 CA MOTA 1.00 28.56 AAGL 17.033 121,351 206 20.060 1609 CB ASP ATOM AAGL 15.871 122.315 1.00 31.99 19.996 206 ASP MOTA 1610 CG 1.00 30.07 AAGL 14.791 121.990 20.539 1611 OD1 ASP 206 MOTA 16.037 123.390 1.00 30.30 AAGL 206 19.385 OD2 ASP 1612 MOTA 1.00 28.75 AAGL 17.986 119.352 21.151 206 MOTA 1613 C ASP AAGL 17.597 118.376 1.00 29.56 20.514 206 Ó ASP 1614 ATOM 1.00 27.57 AAGL 19.217 119.437 21.653 1615 И PHE 207 MOTA 20.147 118.321 1.00 27.18 AAGL 21.496 207 PHE MOTA 1616 CA 1.00 24.79 AAGL 20.315 21.106 118.567 207 1617 CB PHE ATOM 1.00 24.63 AAGL 22.115 119.651 207 20.541 1618 CG PHE MOTA 1.00 26.07 AAGL 21.728 120.981 20.643 CD1 PHE 207 ATOM 1619 23.473 119.341 1.00 26.18 AAGL 20.613 CD2 · PHE 207 1620 MOTA 1.00 23.87 AAGL 22.677 121.986 PHE 207 20.811 CE1 MOTA 1621 AAGL 1.00 24.35 24.433 120.340 20.782 PHE 207 MOTA 1622 CE₂ 1.00 26.22 AAGL 24.032 121.661 20.880 207. PHE 1623 CZ MOTA AAGL 22.767 20.917 117.974 1.00 27.60 MOTA 1624 C PHE 207 AAGL 1.00 28.27 23.700 20.987 118.772 PHE 207 1625 0 ATOM AAGL 21.503 116.780 1.00 28.39 22.784 208 ATOM 1626 N ASP AAGL 22.209 116.278 1.00 28.84 ASP 208 23.958 1627 CA MOTA AAGL 24.329 21.618 114.918 1.00 28.97 208 ATOM 1628 CB ASP 20.102 114.930 AAGL 1.00 29.39 CG ASP 208 24.337 MOTA 1629 AAGL 19.521 115.686 1.00 30.72 25.139 208 ATOM 1630 OD1 ASP 1.00 30.15 AAGL 19.494 114.187 1631 OD2 ASP 208 23.537 ATOM AAGL 1.00 28.85 ASP 23.910 23.737 116.143 208 ATOM 1632 C 1.00 28.49 AAGL 24.418 116.520 ATOM ASP 208 24.866 1633 0 1.00 26.19 AAGL 24.263 115.595 209 22.817 TYR MOTA 1634 N AAGL 22.674 25.704 115.368 1.00 25:08 1635 TYR 209 MOTA CA 1.00 26.01 AAGL TYR 209 22.353 26.001 113.896 MOTA 1636 CB AAGL 25,677 112,854 1.00 23.51 23.397 TYR 209 MOTA 1637 CG AAGL 25.427 113.191 1.00 27.73 24.728 1638 CD1 TYR 209 MOTA AAGL 25.693 25.222 112.194 1.00 27.06 209 1639 CE1 TYR MOTA 1.00 26.41 AAGL 25.705 111.506 23.056 1640 CD2 TYR 209 ATOM AAGL 25.503 110.505 1.00 29.44 24.007 209 MOTA 1641 CE2 TYR 25.267 110.856 1.00 25.86 AAGL 209 25.318 ATOM 1642 CZ TYR AAGL 1.00 26.38 26.244 25.103 109.853 209 1643 OH TYR ATOM 1.00 23.78 AAGL 26.398 116.163 209 21.578 TYR ATOM 1644 C AAGL 1.00 23.59 25.774 116.589 209 20.611 ATOM 1645 Q TYR AAGL 27.711 116.315 1.00 25.60 21.745 1646 PHE 210 ATOM N AAGL 1.00 24.58 28.584 116.969 210 20.775 ATOM 1647 CA PHE AAGL 29.576 117.918 1.00 25.18 21.441 1648 СB PHE 210 MOTA AAGL 1.00 26.35 29.004 119.234 21.826 PHE 210 ATOM 1649 CG 28.309 120.004 1.00 26.01 AAGL 20.895 210 1650 CD1 PHE ATOM 1.00 26.73 **AAGL** 29.214 119.741 210 23.104 ATOM 1651 CD2 PHE AAGL 1.00 28.08 27.836 121.269 21.234 210 ATOM 1652 CE1 PHE 1,00 29.00 AAGL 23.453 28.746 121.000 210 MOTA 1653 CE2 PHE 1.00 28.84 AAGL 28.057 121.768 210 22.519 ATOM 1654 ÇZ PHE 1.00 25.37 AAGL 20.167 29.402 115.842 PHE 210 MOTA 1655 С 29.932 115.005 1.00 26.01 AAGL 20.894 PHE 210 ATOM 1656 0 AAGL 1.00 22.48 18.845 29.514 115.817 211 ATOM 1657 N GLY AAGL 1.00 21.15 30.313 114.784 211 18.214 ATOM 1658 CA GLY 1.00 20.32 AAGL 31.333 115.441 17.305 GLY 211 ATOM 1659 C 1.00 22.35 AAGL 31.007 116.412 16.631 MOTA 1660 0 GLY 211 1.00 20.60 AAGL 32.560 114.931 17.285 VAL 212 ATOM 1661 N 1.00 19.19 AAGL 33.595 115.501 16.428 MOTA 1662 CA VAL 212 1.00 20.57 AAGL 34.592 116.400 VAL 212 17.206 CB ATOM 1663

Fig. 3 cont.

17.920 33.859 117.512 1.00 21.04 AAGL CG1 VAL 212 1664 · ATOM 1.00 22.31 AAGL 35.419 115.554 18.169 MOTA 1665 CG2 VAL 212 34.426 114.410 1.00 19.78 AAGL 15.781 VAL 212 С 1666 ATOM: 1.00 19.10 AAGL 16.358 34.616 113.339 212 ATOM 1667 0 VAL 34.914 114.692 AAGL 1.00 18.35 14.581 SER 213 ATOM 1668 N 1.00 19.01 AAGL 13.869 35.775 113.758 213 1669 CA SER MOTA 35.630 113.933 34.305 113.696 1.00 18.11 AAGL 12.353 1670 SER 213 ATOM CB AAGL 1.00 17.61 11.934 213 SER MOTA 1671 OG 37.187 114.148 1.00 18.11 AAGL 14.277 213 MOTA 1672 С SER 1.00 21.77 AAGL 37.461 115.323 14.506 213 SER ATOM 1673 0 AAGL 38.081 113.174 1.00 17.30 14.384 TYR 214 MOTA 1674 N AAGL 1.00 17.43 39.458 113.478 TYR 214 14.744 1675 CA MOTA . AAGL 1.00 19.55 16.252 39.688 113.352 1676 TYR 214 MOTA CB 1.00 18.83 AAGL 41.122 113.624 16.647 1677 TYR 214 CG MOTA AAGL 1.00 22.19 16.558 41.661 114.911 214 1678 CD1 TYR MOTA 43.004 115.158 1.00 22.03 AAGL 16.872 1679 CE1 TYR 214 ATOM AAGL 41.959 112.590 1.00 23.69 17.063 1680 CD2 TYR 214 MOTA 43.307 112.828 1.00 22.60 AAGL CE2 TYR . 214 17.381 MOTA 1681 1.00 22.17 AAGL 17.279 43.816 114.113 214 ATOM 1682 CZ TYR 45.141 114.346 AAGI 1.00 24.19 17.561 214 1683 OH TYR ATOM 1.00 18.48 AAGL 14.013 40.386 112.534 TYR 214 MOTA 1684 С AAGL 1.00 18.33 14.361 40.488 111.358 1685 214 ATOM TYR 41.048 113.067 1.00 18.28 AAGL 12.990 TYR 215 1686 N ATOM 10.717 10.497 10.45 AAGL 1.00 16.96 41.979 112.311 215 ATOM 1687 CA TYR 1.00 16.58 41.506 112.321 AAGL 1688 TYR 215 ATOM CB AAGL 1.00 16.72 40.277 111.465 215 ATOM 1689 CG TYR AAGL 40.377 110.075 1.00 19.62 215 ATOM 1690 CD1 TYR AAGL 1.00 18.54 10.264 39.252 109.274 CE1 TYR 215 MOTA 1691 1.00 16.88 AAGL 10.346 39.013 112.038 215 ATOM 1692 CD2 TYR 1.00 17.19 AAGL 10.156 37.875 111.245 215 MOTA 1693 CE2 TYR AAGL 1.00 16.90 38.007 109.862 10.111 1694 TYR 215 MOTA CZ AAGL 36.910 109.064 1.00 17.46 215 9.868 ATOM 1695 TYR OH AAGI. 43.374 112.920 1.00 19.56 12.297 215 1696 С TYR ATOM AAGL 43.523 114.124 1.00 19.95 215 12.487 1697 0 TYR MOTA 1.00 20.63 AAGL 44.418 112.087 12.184 MOTA 1698 N PRO 216 1.00 20.25 AAGL 44.396 110.613 12,160 216 ATOM 1699 CD PRO 1.00 20.50 45.788 112.589 AAGL 12.308 PRO 216 MOTA 1700 CA AAGL 1.00 22.26 46.476 111.450 PRO 216 13.033 ATOM 1701 CB 1.00 20.29 AAGL 45.881 110.243 12.318 216 1702 CG PRO MOTA 46.503 112.922 AAGL 11.005 1.00 21.80 1703 PRO 216 MOTA 1.00 23.06 AAGL 47.552 113.569 11.021 1704 0 PRO 216 ATOM AAGI. 45.934 112.495 1.00 20.15 9.885 1705 N PHE 217 ATOM AAGL 1.00 19.12 8.599 46.580 112.682 1706 CÀ PHE 217 MOTA AAGL 46.729 111.308 1.00 21.27 7.940 ATOM 1707 CB PHE 217 1.00 22.97 AAGL 45.548 110.390 217 8.166 ATOM 1708 CG PHE 1.00 22.42 AAGL 217 7.783 44.263 110.773 CD1 PHE ATOM 1709 1.00 24.02 AAGL 8.733 45.730 109.129 MOTA 1710 CD2 PHE 217 1.00 22.58 AAGL 7.953 43.177 109.912 CE1 PHE 217 ATOM 1711 AAGL 1.00 22.45 8.910 44.651 108.260 ATOM 1712 CE2 PHE 217 AAGL 1.00 22.51 217 8.518 43.372 108.652 PHE ATOM 1713 CZ. 46.016 113.671 1.00 20.44 AAGL 7.586 PHE 217 MOTA 1714 С AAGL 46.271 113.523 1,00 21.67 0 PHE 217 6.391 1715 MOTA AAGI 45.270 114.676 1.00 22.47 8.040 218 MOTA 1716 N TYR 1.00 23.80 AAGL 44.715 115.688 7.130 1717 TYR 218 CA ATOM AAGL 43,177.115.681 1.00 24.44 218 7.155 TYR MOTA 1718 CB AAGL 1.00 21.12 42.525 114.439 6.583 MOTA 1719 CG TYR 218 1.00 22.80 AAGL 5.331 218 42.891 113.952 CD1 TYR ATOM 1720 1.00 25.22 AAGL 42.281 112.815 4.789 1721 218 ATOM CE1 TYR 1.00 23.62 AAGL CD2 218 7.286 41.528 113.763 TYR MOTA 1722 40.910 112.625 1.00 23.28 AAGL 6.753 CE2 218 ATOM 1723 TYR AAGL 1.00 24.22 CZ. TYR 218 5.504 41.294 112.159 1724 ATOM AAGL 4.970 40.698 111.038 1.00 24.13 1725 TYR 218 MOTA OH 1.00 26.28 AAGL 7.493 45.201 117.089 1726 TYR 218 MOTA C AAGL 1.00 28.68 6.956 44.707 118.087 MOTA 1727 0 TYR 218 1.00 27.77 AAGL 46.163 117.165 8.407 ATOM 1728 N SER 219 AAGL 1.00 28.32 8.854 46.712 118.447 219 MOTA 1729 CA SER 1.00 29.25 AAGL 9.124 45.592 119.457 1730 СВ SER 219 ATOM

## 113/174 AAGL 46.078 120.538 1.00 31.84 9.908 219 SER ATOM 1731 OG 47.549 118.303 1.00 28.53 AAGL 10.119 1732 С SER 219 ATOM AAGL 47.110 117.716 1.00 26.20 219 11.107 1733 SER MOTA 0 AAGL 48.750 118.870 1.00 29.00 10.090 ATOM 1734 N ALA 220 49.647.118.816 1.00 28.92 AAGL CA ALA 220 11.235 MOTA 1735 1.00 28.98 AAGL 51.003 119.371 10.851 220 ALA ATOM 1736 CB 49.104 119.572 1.00 29.06 AAGL ALA 220 12.440 1737 C ATOM 1.00 30.49 AAGL 13.520 49.683 119.507 220 1738 ALA ATOM 0 1.00 29.58 AAGL 12.260: 48.003 120.293 N SER 221 1739 ATOM 1.00 29.31 AAGL 13.358 47.404 121.046 221 ATOM 1740 CA SER 46.522 122.169 1.00 29.65 AAGL 12.815 221 1741 CB SER MOTA 1.00 33.54 AAGL 221 12.148 47,295 123,152 SER ATOM 1742 OG AAGL 46.565 120.160 1.00 27.63 14.278 221 ATOM 1743 C SER 1.00 27.79 AAGL 46.201 120.570 SER 221 15.375 ATOM 1744 0 AAGL 46.264 118.948 1.00 26.73 222 13.828 1745 N ALA ATOM 1.00 25.72 AAGL 45,445 118.017 14.598 ALA 222 MOTA 1746 CA AAGL 44.864 116.953 13.662 1.00 24.78 1747 222 MOTA CB ALA 1,00 26.39 AAGL 46.187 117.347 1748 222 15.764 C ALA MOTA AAGL 1.00 24.72 46.189 116.117 15.889 1749 ALA 222 MOTA 0 46.809 118.157 1.00 25.12 AAGL 16.619 THR 223 ATOM 1750 N AAGL 1.00 26.47 47.536 117.632 223 17.771 1751 CA THR ATOM 48.498 118.678 1.00 26.69 AAGL 223 18.360 1752 THR MOTA CB 1.00 28.21 AAGL 18.793 47.749 119.822 OG1 THR 223 ATOM 1753 AAGL 1.00 25.83 49.520 119.104 17.321 1754 CG2 THR 223 ATOM 1.00 25.83 AAGL 46.573 117.223 18.877 223 1755 C THR MOTA 45,465 117,751 AAGL 1.00 28.38 18.982 1756 THR 223 ATOM 0 AAGL 1.00 26.34 47.000 116.278 19.703 MOTA LEU 224 1757 N AAGL 1.00 27.64 46.177 115.817 20.807 224 1758 CA · LEU MOTA AAGL 46.857 114.647 1.00 30.65 224 21.516 1759 LEU CB ATOM AAGL 1.00 31.90 46.842 113.311 20.769 ATOM 1760 CG LEU 224 47.603 112.257 1.00 32.52 AAGL 21,565 224 1761 CD1 LEU ATOM 1.00 32.19 **AAGL** 224 20.558 45.406 112.873 ATOM 1762 CD2 LEU AAGL 1.00 28.76 45,958 116.967 21.781 1763 LEU 224 MOTA C 1.00 30.90 44.956 117.011 AAGL 22.495 LEU 224 MOTA 1764 0 AAGL 1.00 29.40 21.796 46.902 117.903 1765 N ALA 225 MOTA AAGL 1.00 29.81 46.833 119.070 225 22.663 1766 ALA CA MOTA AAGL 48.163 119.812 1.00 31.20 22.632 225 1767 ÇВ ALA MOTA 45.701 120.013 AAGL 1.00 30.35 225 22.252 ALA ATOM 1768 C AAGL 1.00 29.58 45.003 120.56D 23.105 225 . MOTA 1769 0 ALA 1.00 30.66 45.526 120.215 AAGL 226 20.948 1770 Ŋ SER ATOM 1.00 30.00 AAGL 44.454 121.090 20.472 226 1771 CA SER ATOM 1.00 30.27 AAGL 44.642 121.423 18.995 1772 SER 226 MOTA CB 1.00 34.03 AAGL 18.851 45.426 122.592 226 1773 SER OG ATOM AAGL 43.096 120.437 1.00 27.61 20.685 ATOM 1774 С SER 226 AAGL 42.114 121.113 1.00 27.38 226 21.003 SER 1775 0 MOTA 1.00 26.75 AAGL 20.510 43.053 119.119 227 ATOM 1776 N LEU 41.828 118.359 AAGL 1,00 27.51 1777 LEU 227 20.691 CA ATOM 1.00 25.07 AAGL 20.337 42.060 116.884 227 LEU MOTA 1778 CB 40.857 115.967 1.00 24.78 AAGL 20.555 ATOM 1779 CG LEU 227 1.00 24.45 AAGL 19.578 39,755 116.340 227 1780 CD1 LEU ATOM 1.00 23.51 AAGL 41.268 114.514 20.374 ATOM 1781 CD2 LEU 227 1.00 28.41 AAGL 227 22.148 41.407 118.465 LEU С ATOM 1782 1.00 28.87 AAGL 40.253 118.726 22.456 ATOM 1783 0 LEU 227

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23.037

24.474

25.201

26.700

27.242

26.876

27,322

24.820

25.538

24.299

24.553

23.981

24.783

23.978

Fig. 3 cont.

42.372 118.256

42.132 118.316

43.469 118.150

43.390 117.906

44.757 117.477

45.827 118.489

47.191 118.075

41.485 119.653

40.484 119.710

42.056 120.732

41.532 122.063

42.452 123.142

43.637 123.232

41.748 124.483

1.00 30.45

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1.00 41.65

1.00 43.74

1.00 46.64

1.00 47.80

1.00 30.16

1.00 31.36

1.00 29.71

1.00 30.66

1.00 31.91

1.00 35.38

1.00 34.76

AAGL

						40 - 45 122 202	1.00 30.52	AAGL
ATOM	1798		THR	229	23.973	40.145 122.282	1.00 30.32	AAGL
MOTA	1799	0	THR	229	24.615	39.290 122.883		AAGL
ATOM	1800	N	SER	230		39.932 121.795	1.00 29.88	
MOTA	1801	CA	SER	230	22.077	38.646 121.948	1.00 27.75	AAGL
ATOM	1802	CB	SER	230	20.626	38.766 121.470	1.00 27.43	AAGL '
ATOM	1803	OG	SER	230	19.947	37.532 121.612	1.00 28.20	AAGL
ATOM	1804	С	SER	230	22.790	37.534 121.178	1.00 27.11	AAGL
ATOM	1805	o	SER	230	22.994	36.436 121.698	1.00 27.65	AAGL
ATOM	1806	N	LEU	231	23.157	37.814 119.935	1.00 27.30	AAGL
ATOM	1807	CA	LEU	231	23.859	36.829 119.122	1.00 28.25	AAGL
ATOM	1808	СВ	LEU	231	24.037	37.341 117.687	1.00 28.04	aagl
ATOM	1809	CG	LEU	231	22.767	37.430 116.832	1.00 28.82	AAGL
MOTA	1810		LEU	231	23.091	38.027 115.466	1.00 29.62	AAGL '
ATOM	1811		LEU	231	22.171	36.034 116.670	1.00 25.68	AAGL
ATOM	1812	C	LEU	231	25.228	36.541 119.733	1.00 29.07	AAGL
ATOM	1813	ŏ	LEU	231	25.685	35.399 119.743	1.00 27.21	AAGL
ATOM	1814	И	ALA	232	25.874	37.585 120.244	1.00 30.00	AAGL
	1815	CA	ALA	232	27.198	37,449 120.849	1.00 31.64	AAGL
ATOM		CB	ALA	2.32	27.733	38.828 121.257	1.00 30.69	AAGL
MOTA	1816	С	ALA	232	27.142	36.535 122.063	1.00 31.96	AAGL
ATOM	1817		ALA	232	27.980	35.645 122.229	1.00 32.99	AAGL
MOTA	1818	0	ASN	232	26.146	36.757 122.913	1.00 31.75	AAGL
MOTA	1819	N		233	25.989	35.960 124.118	1.00 33.65	AAGL
MOTA	1820	CA	ASN	233	25.010	36.646 125.071	1.00 33.95	AAGL
MOTA	1821	CB	ASN		25.507	38.010 125.528	1.00 37.26	AAGL
MOTA	1822	CG	ASN	233	26.712	38.267 125.547	1.00 37.11	AAGL
ATOM	1823		ASN	233		38.884 125.912	1.00 37.35	AAGL
MOTA	1824		ASN	233	-24.582 25.558	34.513 123.866	1.00 33.38	AAGL
MOTA	1825	C	ASN	233		33.616 124.621	1.00 34.08	AAGL
MOTA	1826	0	ASN	233	25.932	34.280 122.812	1.00 32.11	AAGL
MOTA	1827	N	LEU	234	24.780	32.927 122.498	1.00 31.75	AAGL
MOTA	1828	CA	LEU	234	24.331		1.00 29.34	AAGL
MOTA	1829	СВ	LEU	234	23.387		1.00 28.94	AAGL
MOTA	1830	CG	LEU	234	21.875	33.038 121.527	1.00 28.45	AAGL
ATOM	1831		LEU	234	21.151	33.301 120.209	1.00 29.20	AAGL
ATOM	1832		LEU	234	21.373	31.739 122.157	1.00 29.20	AAGL
MOTA	1833	C	LEU	234	25.529	32.036 122.200	1.00 31.64	AAGL
MOTA	1834	0	LEU	234	25.651	30.937 122.737	1.00 31.31	AAGL
MOTA	1835	11	GLN	235	26.413	32.530 121.340	1.00 34.83	AAGL
ATOM	1836	CA	GLN	235	27.601	31.797 120.944	1.00 34.48	AAGL
MOTA	1837	CB	GLN	235	28.302	32.560 119.810	1.00 36.34	AAGL
ATOM	1838	CG	GLN	235	29.283	31.756 118.991	1.00 38.22	AAGL
MOTA	1839	CD	GLN	235	30.545	31.410 119.747	1.00 38.29	AAGL
MOTA	1840		GLN	235	31.065	32.224 120.511	1.00 38.23	AAGL
MOTA	1841		GLN	· 235	31.059	30.204 119.521	1.00 35.64	. AAGL
MOTA	1842	С	GLN	235	28.557	31.597 122.122	1.00 33.04	AAGL
ATOM	1843	0	GLN	235	29.063	30.500 122.335	1.00 36.91	AAGL
ATOM	1844	Ŋ	SER	236	28.776	32.659 122.894	1.00 30.91	AAGL
MOTA	1845	CA	SER	236	29.694	32.626 124.034 34.056 124.552		AAGL
MOTA	1846	CB	SER		29.942		1.00 40.94	AAGL
ATOM	1847	OG	SER		28.764	34.620 125.122	1.00 39.31	AAGL
ATOM	1848	¢	SER		29.221			AAGL
MOTA	1849		SER		30.027		1.00 38.31	AAGL
MOTA	1850		THR		27.913			AAGL
MOTA	1851	CA	THR		27.353			AAGL
ATOM	1852				26.002			AAGL
ATOM	1853		1 THR		26.183			AAGL
ATOM	1854		2 THR		25.432			AAGL
MOTA	1855	C	THR		27.169		1.00 36.88	
MOTA	1856		THR		27.503		1.00 37.95	AAGL
MOTA	1857	N	TYR		26.653		1.00 35.86	AAGL
MOTA	1858	CA	TYR		26.391			AAGL
ATOM	1859	СВ	TYR	238	24.955			AAGL
MOTA	1860	CG	TYR	238	23.924			AAGL
ATOM	1861	CD	1 TYR		23.513	27.376 126.125		AAGL
MOTA	1862		1 TYR		22.630			AAGL
ATOM	1863	CD	2 TYR	238	23.416			AAGL
MO'LA	1864	CE	2 TYP	238	22.531	29.961 125.935	1.00 32.31	AAGL

Fig. 3 cont.

					. 11	5/174		
ATOM	1865	CZ	TYR	238	22.146	29.150 126.992	1.00 32.31	AAGL
ATOM	1866	OH	TYR	238	21.291	29.646 127.951	1.00 34.51	AAGL
ATOM	1867	Ċ	TYR	238	27.377	27.210 123.570	1.00 34.17	. AAGL AAGL
MOTA	1868	0	TYR	238	27.327	26.023 123.245	1.00 32.44 1.00 34.59	AAGL
ATOM	1869	N	ASP	239	28.263	28.060 123.060 27.645 122.080	1.00 34.39	AAGL
MOTA	1870	CA	ASP	239 239	29.267 30.292	26.716 122.754	1.00 38.30	AAGL
MOTA	1871 1872	CB CG	ASP ASP	239	31.412	26.290 121.819	1.00 39.89	AAGL
ATOM ATOM	1873	OD1		239	31.811	27.088 120.939	1.00 40.54	aagl
ATOM	1874	OD2		239	31.911	25.155 121.975	1.00 41.25	AAGL
ATOM	1875	С	ASP	239	. 28.688	26.982 120.829	1.00 34.34	AAGL
ATOM	1876	0	ASP	239	29.098	25.885 120.451	1.00 34.85	aagl aagl
MOTA		· N	LYS	240	27.735	27.656 120.190 27.155 118.963	1.00 32.57 . 1.00 31.63	AAGL
MOTA	1878	CA	LYS	240	27.121 ·25.746	26.525 119.234	1.00 .30.18	AAGL
ATOM	1879 1880	CB CG	LYS LYS	· 240 240	25.764	25.264 120.104	1.00 33.39	AAGL
ATOM ATOM	1881	CD	LYS	240	24.367	24.648 120.218	1.00 31.95	· AAGL
ATOM	1882	CE	LYS.	240	24.318	23.502 121.247	1.00 32.26	AAGL
ATOM	1883	NZ	LYS	240	25.241	22.379 120.930	1.00 29.98	AAGL ·
MOTA	1884	C	LYS	240	26.953	28.315 117.990	1.00 29.66	AAGL
MOTA	1885	0	LYS.		. 26.779	29.460 118.400	1.00 30.38 1.00 29.06	AAGL AAGL
ATOM	1886	N	PRO	241	27.010 27.422	28.036 116.679 26.781 116.028	1.00 29.36	AAGL
MOTA	1887 1888	CD	PRO PRO	241 241	26.850	29.106 115.691	1.00 27.35	AAGL
atom Atom	1889	CB	PRO	241	27.136	28.403 114.371	1.00 27.28	· AAGL
MOTA	1890	CG	PRO	241	28.058	27.285 114.768	1.00 29.28	AAGL .
ATOM	1891	C	PRO	241	- 25.434	29.693 115.732	1.00 28.09	AAGL
ATOM	1892	0	PRO	241	24.491	29.048 116.201	1.00 27.43	AAGL
MOTA	1893	N	VAL	242	25.294	30.911 115.225	1.00 27.44 1.00 27.37	aagl aagl
ATOM	1894	CA	VAL	242	24.005	31.588 115.192 32.871 116.015	1.00 27.37	AAGL
MOTA	1895	CB	VAL	242 24 <b>2</b>	24.047 24.156	32.531 117.479	1.00 27.77	AAGL
MOTA MOTA	1896 1897		VAL	242	25.242	33.719 115.588	1.00 27.66	AAGL
ATOM	1898	C	VAL	242	23.614	31.929 113.763	1.00 26.08	AAGL
MOTA	1899	0	VAL	242	24.468	32.140 112.903	1.00 27.26	AAGL
ATOM	1900	N	VAL	243	22,313	31.990 113.512	1.00 25.38	AAGL
MOTA	1901	CA	VAL	243	. 21.806	32.287 112.179	1.00 22.94 1.00 24.38	AAGL AAGL
MOTA .	1902	CB	VAL	243	21.431	30.973 111.419 31.285 109.996	1.00 23.02	AAGL
ATOM	1903 1904		VAL	243 243	20.994 22.612	30.009 111.409	1.00 25.53	
MOTA MOTA	1905	CGZ	VAL	243	20.541	33.129 112.289	1.00 22.55	AAGL
ATOM	1906	ō	VAL	243	19.691	32.836 113.115	1.00 21.01	AAGL
ATOM	1907	N	VAL	.244	20.432	34.188 111.487	1.00 21.40	AAGL
MOTA	1908	CA	VAL	244	19.213	34.995 111.483	1.00 21.25	AAGL
ATOM	1909	CB	VAL	244	19.469	36.463 111.094	1.00 21.49 1.00 22.74	AAGL AAGL
ATOM	1910		LVAL	244	18.139 20.263	37.170 110.884 37.163 112.188	1.00 20.20	AAGL
MOTA MOTA	1911 1912	C	VAL VAL	244 244	18.414	34.309 110.387	1.00 19.60	AAGL
MOTA	1913	õ	VAL		18.720	34.446 109.205	1.00 20.42	AAGL
MOTA	1914	N	VAL		17.395	33.557 110.780	1.00 17.97	AAGL
ATOM	1915	CA	VAL	245	16.635	32.788 109.807	1.00 17.90	AAGL
ATOM	1916	CB	VAL		16.234	31.431 110.413	1.00 18.93	AAGL
MOTA	1917		VAL		17.485	30.699 110.871 31.637 111.578	1.00 18.12 1.00 17.48	AAGL AAGL
ATOM	1918		2 VAL		15.274		1.00 17.48	AAGL
MOTA	1919 1920	C	VAL VAL		15.415 14.783		1.00 17.57	AAGL
MOTA MOTA	1921	N	GLU		15.085			AAGL
ATOM	1922	CA	GLU		13.949	35.392 109.143	1.00 18.02	AAGL
MOTA	1923		GLU		12.657	35.023 109.875	1.00 22.04	AAGL
ATOM	1924	CG	GLU		11.917			AAGL
ATOM	1925				10.611			AAGL AAGL
MOTA	1926		1 GLU		9.882			AAGL
ATOM	1927		2 GLU		10.311 14.163			AAGL
MOTA MOTA	1928 1929		GLU GLU		14.163			AAGL
ATOM	1930		THR		13.912		1.00 17.83	AAGL
ATOM	1931				14.024			AAGL
					Accord to	•		

Fig. 3 cont.

## 116/174 AAGL 39,584 108.487 1.00 21.29 15.505 247 1932 CB THR ATOM 40.968 108.857 AAGL 1.00 22.65 OG1 THR 247 15.532 1933 ATOM 1.00 20.07 AAGL 16.238 39.409 107.172 247 1934 CG2 THR MOTA 39.774 107.167 AAGL 1.00 18.87 1935 C THR 247 13.356 MOTA AAGL 13.167 39,141 106,134 1.00 19.64 247 1936 0 THR ATOM 41.039 107.326 AAGL 1.00 17.13 248 12,980 1937 N ASN ATOM 1.00 18.39 AAGL 248 12.312 41.816 106.281 ATOM 1938 CA ASN 41.800 106.466 1.00 19.04 AAGL 248 10.793 1939 CB ASN MOTA AAGL 1.00 20.07 40.616 105.836 248 10.095 ASN ATOM 1940 CG 40.475 106.007 1.00 23.76 AAGL 1941 OD1 ASN 248 8.889 MOTA 1.00 20.10 AAGL 39.775 105.113 248 10.820 ND2 ASN ATOM 1942 43.291 106.427 1.00 18.69 AAGL 12.685 ASN 248 ATOM 1943 С 1.00 17.33 AAGL 13.135 43.725 107.483 1944 0 ASN 248 MOTA AAGL 44.046 105.355 1.00 19.91 12,466 249 1945 TRP **ATOM** N 1.00 21.18 AAGL 12.630 45.503 105.355 TRP 249 ATOM 1946 CA 1.00 21.42 AAGL 14.065 45.981 105.129 MOTA 1947 CB TRP 249 1.00 19.99 AAGL 47.491 105.288 14.117 TRP 249 ATOM 1948 CG 48.225 106.517 AAGL 1.00 19.73 249 14.261 1949 CD2 TRP MOTA AAGL 1:00 19.65 49.599 106.208 14.108 1950 CE2 TRP 249 ATOM AAGL 14.499 47.853 107.847 1.00 19.37 249 1951 CE3 TRP ATOM AAGL 48.431 104.313 1.00.20.84 249 13.895 1952 CD1 TRP MOTA AAGL 1.00 19.99 49.693 104.861 13.887 ATOM 1953 NE1 TRP 249 1.00 20.08 AAGL 50.604 107.187 14.185 249 1954 CZ2 TRP MOTA 1.00 21.35 AAGL 249 14.575 48.853 108.820 CZ3 TRP MOTA 1955 50.214 108.481 1.00 21.66 AAGL 14.418 ATOM 1956 CH2 TRP 249 1.00 20.70 AAGL 11.722 46.003 104.241 249 1957 TRP MOTA C AAGL 1.00 22.36 11.800 45.539 103.102 MOTA 1958 0 TRP 249 AAGL 1.00 22.00 46.957 104.559 1959 250 10.838 PRO MOTA N 1.00 21.04 AAGL 47.625 105.865 10.686 ATOM 1960 CD PRO 250 AAGL 47.508 103.587 1.00 21.27 250 9.894 1961 CA PRO ATOM 1.00 22.31 AAGL 48.210 104.477 8.876 250 ATOM 1962 CB PRO 1,00 22.64 AAGL 48.783 105.538 250 9.744 ATOM 1963 CG PRO AAGL 10.402 1.00 23.33 48.435 102.507 250 С PRO ATOM 1964 49.268 102.743 1.00 21.79 AAGL 11.270 PRO 250 ATOM 1965 0 AAGL 9.844 48.282 101.311 1.00 23.27 JAV 251 MOTA 1966 N 49.165 100.212 1.00 24.85 AAGL 10.185 MOTA 1967 CA VAL 251 **AAGL** 1.00 24.44 10.171 48.437 98.854 1968 VAL 251 CB MOTA 98.787 1.00 24.31 AAGL 11.335 47.476 VAL 251 MOTA 1969 CG1 AAGL 1.00 28.76 ATOM 1970 CG2 VAL 251 8.865 47.699 98,657 AAGL 9.095 50.227 100.278 1.00 26.42 251 С VAL MOTA 1971 99.646 AAGL 9.177 51.281 1.00 24.68 MOTA 1972 0 VAL 251 AAGL 1.00 27.57 8.075 49.934 101.083 MOTA 1973 N SER 252 1.00 27.22 AAGL 50:851 101.298 6.962 MOTA 1974 ·CA SER 252 1.00 28.72 AAGL 252 5.942 50.722 100.164 1975 SER CB MOTA 1.00 28.82 AAGL 51.662 100.327 4.895 1976 SER 252 MOTA OG AAGL 1.00 28,31 SER 252 6.289 50.558 102.642 1977 С MOTA 5.858 49,434 102.886 1.00 26.39 AAGL ATOM 1978 0 SER 252 1.00 27.82 AAGL 51.559 103.518 ATOM 1979 N CYS 253 6.232 AAGL 1.00 27.19 5.594 51.413 104.824 253 MOTA 1980 CA CYS AAGL 1.00 28.86 52.738 105.201 253 4.932 MOTA 1981 C CYS AAGL 1.00 27.40 5,411 53.436 106.091 253 MOTA 1982 O CYS 51.031 105.913 1.00 27.78 AAGL 6.611 253 MOTA 1983 CB CYS **AAGL** 1.00 28.15 253 5.803 50.369 107.406 SG CYS ATOM 1984 53.089 104.528 1.00 30.47 AAGL 3.812 MOTA 1985 N PRO 254 1.00 30.66 AAGL 3.166 52.222 103.525 CD PRO 254 1986 MOTA 3.022 54.314 104.725 1.00 32.44 AAGL 1987 CA PRO 254 ATOM 1.00 32.43 AAGL 1.739 54.023 103.951 MOTA 1988 CB PRO 254 AAGL 53.171 102.837 1.00 33.11 2.206 ATOM 1989 CG PRO 254 AAGL 1.00 34.76 2.739 54.660 106.181 PRO 254 1990 C ATOM 1.00 35.87 **AAGL** 2.780 55.828 106.570 MOTA 1991 0 PRO 254 1.00 35.37 AAGL 2.429 53.653 106.987 ASN 255 ATOM 1992 N 1.00 36.89 AAGL 53.912 108.392 2.161 1993 CA ASN 255 ATOM AAGL 1.00 37.41 0.755 54.457 108.575 1994 CB ASN 255 ATOM AAGL 1.00 38.46 0.410 54.682 110.030 ASN 255 MOTA 1995 CG **AAGL** 55.124 110.832 1,00 35.39 255 1.254 MOTA 1996 OD1 ASN AAGL 54.389 110.387 1.00 34.81 -0.833 ATOM 1997 ND2 ASN 255 AAGL 52.691 109.263 1.00 35.87 2.354 ASN 255 MOTA 1998 C

Fig. 3 cont.

							1 00 36 70	AAGL
MOTA	1999	0	ASN	255	1.471	51.841 109.375	1.00 36.70 1.00 35.76	AAGL
MOTA	2000	N	PRO	256	3.520	52.601 109.910		
ATOM	2001	CD	PRO	256	4.640	53.550 109.780	1.00 35.85	AAGL
ATOM	2002	CA	PRO	256	3.878	51.493 110.791	1.00 34.93	AAGL .
ATOM	2003	CB	PRO	256	5.387	51.654 110.927	1.00 35.60	AAGL
ATOM	2004	CG	PRO	256	5.558	53.122 110.901	1.00 36.37	AAGL
ATOM	2005	C	PRO	256	3.158	51.543 112.140	1.00 34.50	AAGL
ATOM		٠٥	PRO	256	3.041	52.604 112.752	1.00 33.71	AAGL
	.2007	N	ALA	257	2.683	50.393 112.603	1.00 32.93	AAGL
ATOM	200B	CA	ALA	257	1.988	50.327 113.880	1.00 31.85	AAGL
ATOM	2009	CB	ALA	257	1.371	48.946 114.079	1.00 31.01	AAGL
	2010	C	ALA	257	2.970	50.621 115.000	1.00 32.12	AAGL
ATOM			ALA	257	2.591	51.139 116.046	1.00 31.82	AAGL
ATOM	2011	0		258	4.237	50.291 114.771	1.00 31.15	AAGL
ATOM	2012	N	TYR		5.279	50.504 115.761	1.00 32.72	AAGL
ATOM	2013	CA	TYR	258	5.892	49.168 116.169	1.00 35.88	AAGL
atom	2014	CB	TYR :	258		48.226 116.880	1.00 38.05	AAGL
MOTA	2015	CG	TYR	258	4.954		1.00 33.63	AAGL
MOTA	2016		TYR	258	4.136	47.341 116.170	1.00 40.53	AAGL
MOTA	2017		TYR	258	3.276	46.468 116.840	1.00 40.33	AAGL
MOTA	2018		TYR	258	4.889	48.216 118.267		AAGL
MOTA	2019	CE2	TYR	258	4.039	47.357 118.943	1.00 41.64	AAGL
MOTA	2020	CZ	TYR	258	3.236	46.489 118.232	1.00 42.48	
MOTA	2021	OH	TYR	258	2.386	45.659 118.934	1.00 45.83	AAGL
ATOM	2022	С	TYR	258	6.414	51.411 115.293	1.00 32.44	AAGL
MOTA	2023	0	TYR	258	6.736	51.468 114.108	1.00 31.27	AAGL
MOTA	2024	N	ALA	259	7.021	52.121 116.237	1.00 30.79	AAGL
ATOM	2025	CA	ALA	259	8.147	52.983 115.919	1.00 31.35	AAGL
ATOM	2026	CB	ALA	259	8.479	53.864 117.118	1.00 33.39	AAGL
MOTA	2027	C	ALA	259	9.315	52.046 115.607	1.00 29.93	AAGL
ATOM	2028	0	ALA	259	9.458	51.004 116.242	1.00 29.16	AAGL
MOTA	2029	N	PHE	260	10.137	52.392 114.623	1.00 29.81	AAGL
ATOM	2030	CA	PHE	260	11.281	51.548 114.285	1.00 29.03	AAGL
ATOM	2031	CB	PHE	260	11.772	51.871 112.867	1.00 28.71	AAGL
MOTA	2032	CG	PHE	260	11.007	51.157 111.776	1.00 29.00	AAGL
	2032		PHE	260	9.622	51.242 111.704	1.00 29.61	AAGL
MOTA	2033	CD2		260	11.676	50.379 110.840	1.00 28.02	AAGL
ATOM	2035	CE1		260	8.915	50.558 110.720	1.00 30.59	AAGL
MOTA	2036	CE2		260	10.979	49.694 109.854	1.00 29.46	AAGL
ATOM			PHE	260	9.594	49.783 109.796	1.00 29.30	AAGL
ATOM	2037	CZ		260	12.409	51.765 115.300	1.00 29.23	AAGL
MOTA	2038	C	PHE	260	12.464	52.806 115.957	1.00 29.38	AAGL
ATOM	2039	0	PHE		13.302	50.771 115.466	1.00 29.34	AAGL
MOTA	2040	N	PRO	261		49.414.114.891	1.00 29.47	. AAGL
MOTA	2041	CD	PRO	261	13.247	50.891 116.409	1.00 29.63	AAGL
MOTA	2042	CA	PRO	261	14.418	49.599 116.186	1.00 28.18	AAGL
ATOM	2043	CB	PRO	261	15.194	48.617 115.852	1.00 28.51	AAGL
MOTA	2044	CG	PRO	261	14.096	52.137 116.063	1.00 29.95	AAGL
ATOM	2045	C	PRO	261	15.240	52.539 114.897	1.00 30.37	AAGL
ATOM	2046	0	PRO	261	15.312			AAGL
MOTA	2047	N	SER	262	15.846	52.736 117.082	1.00 32.41 1.00 31.88	AAGL
Mota	2048	CA	SER	262	16.637	53.951 116.922	1.00 33.67	AAGL
MOTA	2049	CB	SER	262	17.167	54.396 118.291		AAGL
MOTA	2050	OG	SER	262	17.708	53.295 119.003	1.00 37.49	AAGL
ATOM	2051	C	SER	262	17,785	53.858 115.918	1.00 32.30	
MOTA	2052	0	SER	262	17.967	54.773 115.107	1.00 32.95	AAGL
MOTA	2053	N	ASP	263	18.565	52.778 115.955	1.00 31.17	AAGL
MOTA	2054	ÇA	ASP	263	19.660	52.663 115.000	1.00 31.60	AAGL
ATOM	2055	ÇB	ASP	263	20.768	51.724 115.512	1.00 31.48	AAGL
MOTA	2056	CG	ASP	263	20.241	50.418 116.090	1.00 31.74	AAGL
ATOM	2057		1 ASP		19.111	49.994 115.748	1.00 30.33	AAGL
ATOM	2058		2 ASP		20.987	49.796 116.887	1,00 30.41	AAGL
ATOM	2059		ASP		19.210		1.00 31.45	AAGL
ATOM	2060		ASP		20.036		1.00 32.04	AAGL
ATOM	2061		LEU		17.905		1.00 30.59	AAGL
ATOM	2062		LEU		17.363			AAGL
ATOM	2063		LEU		16.621		1.00 27.83	AAGL
ATOM	2064	CG			17,375			AAGL
			1 LEU		16.389			AAGL
ATOM	2065	CD.	- 750	204	40.509			

Fig. 3 cont.

MOTA	2066	CD2	LEU	264	18.429	48.955 1		1.00 27.53	AAGL
	2067	c	LEU	264	16.391	52.971 1	11.512	1.00 28.95	AAGL
MOTA			LEU	264	15.941	52,893		1.00 27.43	AAGL
MOTA	2068	-		265	16.074	53,965		1.00 30.75	AAGL
MOTA	2069	И	SER			54.986		1.00 32.24	AAGL
MOTA	2070	CA .	SER	265	15.120			1.00 33.67	AAGL
ATOM	2071	CB	SER	265	14.662	55.779			
MOTA	2072	OG	SER	265	15.763	56.287		1.00 34.70	AAGL'
ATOM	2073	С	SER	265	15.572	55,941		1.00 33.25	AAGL
ATOM	2074	ō	SER	265	14.776	56.742	110.328	1.00 34.94	aagl
	2075	N	SER	266	16.832	55.859	110.399	1.00 33.96	AAGL
ATOM				266	17.305	56.745	109.339	1.00 33.28	AAGL
MOTA	2076	CA	SER			57.133	109 576	1.00 34.74	AAGL
ATOM	2077	CB	SER	266	18.765	56.107	100 142	1.00 40.32	AAGL
MOTA	2078	OG .	SER	266	19.652			1.00 31.87	AAGL
ATOM	2079	С	SER	266	17.176	56.085			AAGL
ATOM	2080	0	SER	266	17.236	56.754		1.00 30.82	
MOTA	2081	N	ILE	267	16.982	54.773		1.00.28.10	AAGL
ATON.	2082	CA	ILE	267	16.874	54.025	106.713	1.00 26.55	AAGL
ATOM	2083	CB	ILE	267	17.067	52.523	106.983	1.00 25.69	· AAGL
	2084		ILE	267	17.120		105.666	1.00 26.74	<b>AAGL</b>
ATOM		CGZ	TIE	267	18.349		107.801	1.00 28.70	AAGL.
ATOM ·	2085		ILE		18.606		108.250	1.00 27.91	. AAGL
ATOM	2086		ILE	267			106.024	1.00 25.54	AAGL
MOTA	2087	С	ILE	267	15.537			1.00 24.26	AAGL
MOTA	2088	0	ILE	267	14.482		106.604		AAGL
MOTA	2089	N	PRO	268	15.567		104.767	1.00 25.09	
MOTA	2090	CD	PRO	268	16.725	55.097	103.932	1.00 26.35	AAGL
ATOM	2091	CA	PRO	268	14.312	54.986	104.058	1.00 25.07	AAGL
ATOM	2092	СВ	PRO	268	14.767	55.792	102.844	1.00 26.89	AAGL
	2093	CG	PRO	268	16.108		102.560	1.00 26.87	AAGL
MOTA			PRO	268	13.602		103.662	1.00 24.21	AAGL
ATOM	2094	C			14.208		103.644	1.00 23.10	AAGL
ATOM	2095	0	PRO	268			103.362	1.00 23.20	' AAGL
ATOM	2096	N	PHE	269	12.313			1.00 23.46	AAGL
ATOM	2097	CA	PHE	269	11.525		102.931		AAGL
MOTA	2098	CB	PHE	269	10.091		103.446	1.00 24.32	
MOTA	2099	CG	PHE	269	9.994		104.942	1.00 24.64	AAGL
MOTA	2100	CD1	PHE	269	10.819		105.758	1.00 25.88	AAGL
ATOM	2101	CD2	PHE	269	9.070	53.706	105.535	1.00 25.95	AAGL
ATOM	2102		PHE	269	10.722	52.168	107,151	1.00 26.08	AAGL
ATOM	2103		PHE	269	8.965	53.788	106.925	1.00 23.79	AAGL
	2104	CZ	PHE	269	9.793		107.732	1.00 23.02	AAGL
ATOM				269	11.548		101.413	1.00 23.22	AAGL
MOTA	2105	C	PHE		10.778		100.774	1.00 23.95	AAGL
MOTA	2106	0	PHE	269			100.848	1.00 23.29	AAGL
ATOM	2107	N	SER	270	12.462			1.00 24.41	AAGL
ATOM	2108	CA	SER	270 .	12.649	51.848	99.410		AAGL
MOTA	2109	CB	SER	270	13.282	53.140		1.00 24.90	
ATOM	2110	OG	SER	270	14.547	53.300		1.00 25.23	AAGL
ATOM	2111	С	SER	270	13.596	50.702		1.00 22.81	AAGL
ATOM	2112	0	SER	270	14.147	50.105	100.055	1.00 25.01	AAGL
ATOM	2113	N	VAL		13.791	50.392	97.845	1.00 23.71	AAGL
	2114	CA	VAL		14.702	49.316	97.477	1.00 22.85	AAGL
ATOM				271	14.846	49.170		1.00 24.85	AAGL
ATOM	2115	CB	VAL	_	15.953	48.172		1.00 23.46	AAGL
MOTA	2116		1 VAL					1.00 22.67	AAGL
ATOM	2117		2 VAL		13.534	48.698			AAGL
ATOM	2118	С	VAL	271	16.065	49.649			
ATOM	2119	0	VAL	271	16.744	48.787			AAGL
ATOM	2120	N	ALA	272	16.453	50.914	97.932		AAGL
ATOM	2121				17.740	51.373			AAGL
MOTA	2122				17.946	52.858	98.104	1.00 26.33	AAGL
ATOM	2123		ALA		17.814				AAGL
					18.839		100.479		AAGL
MOTA	2124		ALA		16.722		100.646		AAGL
ATOM	2125		GLY						AAGL
ATOM	2126				16.710		102.086		AAGL
MOTA	2127	C	GLY		16.808	49.814	102.448	1.00 21.98	AAGL
ATOM	2128	0	GLY		17.427		103.443		
ATOM	2129		GLN		16.192	48.973	101.623	1.00 23.13	AAGL
ATOM	2130				16.210	47.534	101.837	1.00 23.82	AAGL
MOTA	2131				15.354	46.862	2 100.770	1.00 26.47	AAGL
ATOM	2132				14.976	45.429	101.049		AAGL
MULL	Z132	. ,,,	اللت	~ ( 3	_3.510				

Fig. 3 cont.

119/174 AAGL 44.926 100.034 1.00 29.11 13.969 274 2133 ATOM CD GLN 98.846 1.00 26.58 AAGL 44.819 14.273 ATOM 2134 OEl GLN 274 44.630 100.491 AAGL 1.00 22.87 274 12.760 NE2 GLN ATOM 2135 AAGL 47.047 101.741 1.00 24.42 17.655 2136 C GLN 274 MOTA 46.184 102.500 AAGL 1,00 23.54 274 18.090 GLN ATOM 2137 0 AAGL 47.621 100.807 1.00 22.92 18.405 GLN 275 ATOM 2138 N AAGL 47.240 100.627 1.00 22.23 275 19.802 CA GLN ATOM 2139 AAGL 47.863 99.349 1.00 25.17 20.347 GLN 275 ATOM 2140 CB 98.089 AAGL 1.00 25.16 19.668 47.370 ÇG GLN 275 2141 MOTA AAGL 1.00 29.65 20.162 48.099 96.862 275 ATOM 2142 CD GLN 96.677 1.00 33.06 AAGL 49.283 275 19.879 2143 OE1 GLN MOTA AAGL 1.00 30.34 20.915 47.403 96.021 GLN 275 2144 NE2 MOTA AAGL 47.679 101.807 1.00 22.46 2145 275 20.658 MOTA C GLN AAGL 46.924 102.289 1.00 23.14 275 21.492 GLN MOTA 2146 0 AAGL 48.906 102.268 1.00 23.39 276 20.444 ATOM 2147 N GLU 1.00 22.93 AAGL 21.203 49,448 103.386 GLU 276 MOTA 2148 CA AAGL 20.821 50.917 103.615 1.00 26.77 GLU 276 MOTA 2149 CB 1.00 31.09 AAGL 51.518 104.891 276 21.393 2150 GLU MOTA CG AAGL 1.00 33.52 21.007 52.982 105.081 276 2151 GLU MOTA CD 1.00 35.95 AAGL 53.402 104.533 19.968 GLU 276 2152 OE1 MOTA AAGL 1.00 34.45 53.704 105.791 276 21.734 ATOM 2153 OE2 GLU AAGL 48.620 104.643 1.00 23.86 2154 276 20.948 GLU ATOM С 1.00 22.86 AAGL 48.302 105.385 21.870 GLU 276 ATOM 2155 0 AAGL 1.00 22.41 48.261 104.876 19.692 ATOM 2156 N PHE 277 1.00 21.05 AAGL 47.458 106.042 277 19.355. PHE MOTA 2157 CA AAGL 47.222 106.120 1.00 20.89 17.844 2158 PHE 277 ATOM CB 1.00 19.02 AAGL 46.219 107.171 2159 17.447 PHE 277 ATOM CG AAGL 46.533 108.518 1.00 21.55 17.541 277 2160 CD1 PHE MOTA ·AAGL 44.946 106.805 1.00 22.72 17.003 CD2 PHE 277 MOTA 2161 AAGL 1.00 23.87 45.594 109.498 17.200 2162 CE1 PHE 277 ATOM AAGL 43.998 107.781 1.00 21.01 277 1.6.660 ATOM CE2 PHE 2163 1.00 22.10 AAGL 16.759 44.323 109.122 277 ATOM 2164 CZPHE 46.102 105.989 1.00 20.46 AAGL 277 20.051 MOTA 2165 С PHE 1.00 20.12 AAGL 20.676 45.674 106.952 277 PHE ATOM 2166 0 AAGL 45.421 104.856 1.00 20.92 LEU 278 19.928 MOTA 2167 N 1.00 23.04 AAGL 44.107 104.716 20.541 LEU 278 2168 CA MOTA 1.00 24.67 AAGL .20.225 43.512 103.340 2169 CB LEU 278 MOTA AAGL 1.00 24.46 278 18.764 43.076 103.160 MOTA 2170 LEU CG 1.00 26.14 AAGL 42.589 101.741 18.548 278 ATOM 2171 CD1 LEU 1.00 26.55 AAGL 41.964 104.161 278 18.427 2172 CD2 LEU ATOM .AAGL 22.040 1.00 23.23 44.144 104.947 LEU 278 MOTA 2173 С 43.273 105.615 1.00 20.93 AAGL LEU 278 22.593 ATOM 2174 0 1.00 24.22 AAGL 22.707 45.155 104.404 279 GLU 2175 MOTA N 45.244 104.601 1.00 25.09 **AAGL** ATOM 2176 CA GLU 279 24.141 1.00 26.59 AAGL 24.735 46.309 103.682 279 GLU ATOM 2177 CB 1.00 32.07 AAGL 46.045 102.213 24.418 279 MOTA 2178 CG GLU 1.00 37.00 AAGL GLU 279 25.419 46.691 101.274 2179 CD ATOM AAGL 47.815 101.576 1.00 39.68 25.859 279 ATOM 2180 OE1 GLU AAGL 46.078 100.235 1.00 40.09 MOTA 2181 OE2 GLU 279 25.756 AAGL 45.537 106.062 1.00 23.19 279 24.460 GLU ATOM 2182 C 44.984 106.614 AAGL 1.00 23.97 25.409 MOTA 2183 0 GLU 279 1.00 24.51 AAGL 280 23.669 46.391 106.701 LYS MOTA 2184 N 1.00 24.24 AAGL 46.688 108.105 23.922 ATOM 2185 CA LYS 280 1.00 25.42 AAGL 280 23.076 47.879 108.566 LYS MOTA 2186 CB 1.00 30.50 AAGL 23.535 49.186 107.912 LYS 280 ATOM 2187 CG 1.00 35.06 AAGL CD LYS 280 22.847 50.429 108.463 ATOM 2188 AAGL 23.561 51.683 107.932 1.00 38.33 2189 CE LYS 280 MOTA AAGL 1.00 39.58 52.962 108.460 280 23.003 2190 NZ LYS ATOM 45.458 108.975 AAGL 23.665 1.00 24.77 ATOM 2191 С LYS 280 1.00 21.68 AAGL 45.219 109.949 280 24.382 2192 0 LYS MOTA AAGL 22.655 44.669 108.614 1.00 23.74 281 2193 N LEU MOTA 1.00 23.71 AAGL 43,449 109.365 2194 22.351 MOTA ÇA LEU 281 AAGL 42.844 108.891 1.00 21.53 21.023 LEU 281 MOTA 2195 CB 41.484 109.478 1.00 21.28 AAGL LEU 281 20.603 MOTA 2196 CG AAGL 1.00 19.24 41.533 110.996 CD1 LEU 281 20.583 MOTA 2197 AAGL 41.109 108.937 1.00 19.79 CD2 LEU 281 19.226 MOTA 2198 1,00 22.36 AAGL 23.482 42,429 109.172 LEU 281 MOTA 2199 C

Fig. 3 cont.

## 120/174 41.803 110.125 AAGL 1.00 24.16 23.940 LEU 281 MOTA 2200 0 42.267 107.928 1.00 23.73 AAGL 23.921 282 ALA ATOM 2201 N AAGL 1.00 23.94 41.339 107.611 24.998 ATOM 2202 CA ALA 282 41.356 106.120 1.00 23.77 AAGL 25.272 ALA 282 ÇВ 2203 **ATOM** AAGL 1.00 24.05 41.713 108.382 26.264 MOTA 2204 C ALA 282 40.848 108.741 1.00 25.21 AAGL 282 27.060 ALA 2205 0 ATOM AAGL 43.005 108.643 1.00 25.21 26.441 283 ALA MOTA 2206 N 43.477 109.372 AAGL 1.00 25.75 2207 CA ALA 283 27.614 MOTA AAGL 1.00 26.48 27..616 45.005 109.424 283 MOTA 2208 CB ALA 42,898 110.786 AAGL 1.00 26.18 27.635 ATOM 2209 C ALA 2B3 1.00 25.57 AAGL 283 28.658 42.387 111.248 ALA 2210 ATOM O AAGL 42.963 111.465 1.00 25.74 26,493 MOTA 2211 N VAL 284 1.00 25.11 AAGL 42.438 112.824 284 26.383 · CA VAL 2212 MOTA AAGL 42.711 113.414 1.00 24.63 284 24,972 2213 VAL ATOM CB AAGL 41.992 114.744 1.00 24.88 CG1 VAL 284 24.806 2214 ATOM AAGL 24.779 44.220 113.606 1.00 27.53 284 MOTA 2215 CG2 VAL 40.941 112,857 1.00 23.65 AAGL 26.658 MOTA 2216 C VAL 284 AAGL 1.00 23.12 27.416 40.456 113.694 VAL 284 ATOM 2217 0 AAGL 26.052: 40.209 111.930 1.00 25,11 VAL 285 ATOM 2218 N 1.00 23.69 AAGL 38.769 111.881 VAT. 285 26.236 2219 CA MOTA AAGL 38.135 110.839 1.00 24.54 25.302 2220 CB VAL 285 ATOM 36.626 110.822 AAGL 1.00 25.86 25.490 2221 CG1 VAL 285 ATOM AAGL 1.00 26.53 23.855 38,490 111,171 MOTA 2222 CG2 VAL 285 38.406 111.559 1.00 26.05 AAGL VAL 285 27.679 ATOM 2223 C 1.00 25.09 AAGL VAL 285 28.256 37.514 112.179 ATOM 2224 0 AAGL 1.00 24.87 39.101 110.587 28.259 2225 GLU 286 MOTA N 1.00 26.91 AAGL 38.847 110.201 29.639 GLU 286 2226 MOTA CA AAGL 39.737 109.025 30.041 1.00 29.06 286 2227 GLU MOTA CB 39.586 108.629 1.00 32.60 AAGL 31.518 MOTA 2228 CG GLU 286 1.00 35.44 AAGL 38.250 107.971 286 31.812 MOTA 2229 CD GLU 38.120 106.751 1.00 36.64 AAGL 2230 286 31.578 OE1 GLU MOTA AAGL 1.00 35.13 32.264 37.322 108.672 OE2 GLU 286 2231 MOTA AAGL 30.587 39.110 111.367 1.00 26.68 2232 GLU 286 MOTA C 1.00 27.24 AAGL 38.354 111.590 31.528 ATOM 2233 a GLU 286 AAGL 1.00 25.24 40.181 112.111 30.343 287 2234 N ALA MOTA 40.522 113.230 1.00 27.43 AAGL 287 31.211 ATOM 2235 ALA CA AAGL 1.00 27.81 41.990 113.600 287 31.032 MOTA 2236 CB ALA 1.00 29.71 AAGL , 31.003 39.650 114.465 287 2237 C ALA ATOM 1.00 31.32 AAGL 287 31.726 39.795 115.451 ALA MOTA 2238 0 30.024 AAGL 1.00 28,83 38.749 114.415 ATOM 2239 N THR 288 1.00 29.55 AAGL 37.871 115.549 29.744 288 2240 CA THR ATOM AAGL 1,00 28.36 288 28.242 37.499 115.618 2241 CB THR ATOM AAGL 1.00 29.45 38.680 115.459 288 27.444 MOTA 2242 OG1 THR AAGL 1.00 31.36 36.854 116.962 .27.921 288 2243 CG2 THR ATOM 36.577 115.393 1.00 27.55 AAGL 288 30.533 2244 С THR ATOM 1.00 27.21 AAGL 30.708. 36.094 114.280 288 THR ATOM 2245 0 AAGL 31.006 36.015 116.504 1.00 30.08 289 2246 N THR ATOM AAGL 34.770 116.437 1.00 31.68 289 31.757 CA THR ATOM 2247 AAGL 1.00 34.06 34.384 117.806 32,352 289 2248 CB THR MOTA AAGL 35.449 118.291 1.00 35.86 289 33.186 OG1 THR 2249 MOTA 1.00 34.89 AAGL 33.128 117.673 33,186 2250 CG2 THR 289 MOTA 1.00 33.04 AAGL 33.659 115.964 289 30.817 2251 С THR ATOM 1.00 34.14 AAGL 33.332 116.632 29.842 289 ATOM 2252 0 THR AAGL 33.085 114.807 1.00 33.28 31.120 2253 N ASP 290 MOTA AAGL 1.00 32.82 30.298 32.030 114.211 290 ASP MOTA 2254 CA AAGL 1.00 33.97 30.183 30.812 115.137 2255 ASP 290 MOTA CB AAGL 1.00 38.26 29.900 115.054 ATOM 290 31.397 2256 CG ASP AAGL 32.093 29.921 114.006 1.00 38.79 290 MOTA 2257 160 ASP 1.00 38.34 AAGL 290 31.651 29.152 116.024 2258 OD2 ASP ATOM AAGL 1.00 30.86 28.903 32.495 113.793 290 MOTA 2259 C ASP 1.00 31.04 AAGL 31.781 113.979 ASP 290 27.909 ATOM 2260 0 1.00 30.92 AAGL 291 28.841 33.705 113.246 GLY MOTA 2261 N 1.00 28.36 AAGL 34.240 112.740 27.590 GLY 291 MOTA 2262 CA 1.00 28.69 AAGL 27.579 33.689 111.331 291 С GLY MOTA 2263 AAGL 1.00 29.95 28.358 34.133 110.487 MOTA 2264 0 GLY 291 AAGL 1.00 25.52 26.702 32.726 111.065 292 N LEU MOTA 2265 AAGL

Fig. 3 cont.

26.662

292

MOTA

2266

CA

LEU

32.072 109.767

1.00 25.89

					1 44		1.00 25.46	AAGL
ATOM	2267	CB	LEU	292	26.184	30.632 109.940	1.00 25.46	AAGL
MOTA	2268	CG	LEU	292	27.072	29.798 110.858		
ATOM	2269	CD1	LEU	292		28.354 110.807	1.00 26.92	AAGL
MOTA	2270	CD2	LEU	292	28.526	29.929 110.418	1.00 27.08	AAGL
ATOM	2271	С	LEU	292	25.908	32,700 108.613	1.00 25.35	AAGL
MOTA	2272	0	LEU	292	25.298	32.528 107.459	1.00 25.52	AAGL
ATOM	2273	N	GLY	293	24.824	33.413 108.887	1.00 25.75	AAGL
MOTA	2274	CA	GLY	293	24.118	33.990 107.769	1.00 22.89	AAGL
MOTA	2275	С	GLY	293	22.785	34.642 108.043	1.00 23.42	AAGL
MOTA	2276	0	GLY	293	22.366	34.828 109.187	1.00 21.61	AAGL
MOTA	2277	N	VAL	294	22.123	34.984 106.950	1.00 21.14	AAGL
MOTA	2278	CA	VAL	294	20.841	35.647 107.003	1.00 22.60	AAGL
ATOM	2279	CB	VAL	294	21.013	37.164 106.775	1.00 24.33	AAGL
ATOM	2280	CG1	VAL	294	19.657	37.818 106.538	1.00 25.68	AAGL
MOTA	2281	CG2	VAL	294	21.719	37.789 107.969	1.00 23.35	AAGL
ATOM	2282	C	VAL	294	19.926	35.094 105.932	1.00 23.50	AAGL
MOTA	2283	0	VAL	294	20.351	34.867 104.799	1.00 22.80	AAGL
ATOM	2284	N	TYR	295	18.668	34.871 106,293	1.00 21.62	AAGL
ATCM	2285	ÇA	TYR	295	17.684	34.387 105.338	1.00 20.32	AAGL
ATOM	2286	CB	TYR	295	17.105	33.035 105.761	1.00 20.96	AAGL
ATOM	2287	CG	TYR	295	18.040	31.862 105.606	1.00 21.66	AAGL
ATOM	2288		TYR	295	19.124	31.692 106.461	1.00 20.77	AAGL
ATOM	2289		TYR	295	19.974	30.584 106.337	1.00 22.52	AAGL
ATOM	2290		TYR	295	17.820	30.904 104.617	1.00 21.20	AAGL
ATOM	2291		TYR	295	18.658	29.798 104.481	1.00 22.01	AAGL
ATOM	2292	CZ	TYR	295	19.732	29.640 105.341	1.00 22.76	AAGL
ATOM	2293	OH	TYR	295	20.564	28.543 105.211	1.00 23.00	AAGL
ATOM	2294	C	TYR	295	16.554	35.399 105.295	1.00 21.79	AAGL
ATÓM	2295	ŏ	TYR	295	15.933	35.672 106.325	1.00 20.79	AAGL
ATOM	2296	N	TYR	296	16.296	35.966 104.118	1.00 20.08	AAGL
ATOM	2297	CA	TYR	296	15.212	36.927 103.975	1.00 19.64	AAGL
MOTA	2298	CB	TYR	296	15.328	37.704 102.666	1.00 20.6 <del>9</del>	AAGL
ATOM	2299	ÇG	TYR	296	14.503	38.972 102.656	1.00 19.70	AAGL
MOTA	2300		TYR	296	15.005	40.152 103.194	1.00 21.48	AAGL
ATOM	2301		TYR	296	14.236	41.310 103.232	1.00 21.48	AAGL
ATOM	2302		TYR	296	13.203	38.980 102.147	1.00 19.37	AAGL
ATOM	2303	CE2		296	12.423	40.138 102.182	1.00 21.23	AAGL
ATOM	2304	CZ	TYR	296	12.948	41.295 102.729	1.00 20.28	AAGL
ATOM	2305	ОН	TYR	296	12.177	42.427 102.797	1.00 19.16	AAGL
ATOM	2306	С	TYR	296	13.947	36.090 103.939	1.00 20.23	AAGL
ATOM	2307	o	TYR	296	13.945	35.010 103.359	1.00 22.11	AAGL
ATOM	2308	N	TRP	297	12.868	36.578 104.538	1.00 17.43	AAGL
ATOM	2309	CA	TRP	297	11.641	35.795 104.553	1.00 17.69	AAGL
ATOM	2310	СВ	TRP	297	10.942	35.894 105.920	1.00 19.08	AAGL
ATOM	2311	CG	TRP	297	9.854	34.864 106.075	1.00 19.30	AAGL
ATOM	2312		2 TRP	297	8.440	35.098 106.104	1.00 19.62	AAGL
ATOM	2313	CE		297	7.808	33.837 106.201		aagl
ATOM	2314		3 TRP	297	7.644	36.250 106.057	1.00 21.65	AAGL
MOTA	2315		I TRP	297	10.018	33.511 106.155		AAGL
ATOM	2316		TRP	297	8.793	32.885 106.231	1.00 21.42	AAGL
ATOM	2317		2 TRP		6.418		1.00 19.44	<b>AAG</b> L
ATOM	2318		3 TRP		6.257	36.109 106.106	1.00 24.11	aagl
ATOM	2319		2 TRP		5.661	34.836 106.201	1.00 22.67	<b>AAGL</b>
ATOM	2320	C	TRP		10.647			AAGL
ATOM	2321	ŏ	TRP		10.158		1.00 17.76	AAGL
ATOM	2322	N	GLU		10.357			AAGL
MOTA	2323				9.391			AAGL
	2324	CB			7.976			AAGL
MOTA	2325				7.562			AAGL
ATOM					7.283			AAGL
MOTA	2326		GLU 1 GLU		7.320			AAGL
ATOM	2327				7.016			AAGL
MOTA	2328		2 GLU		9.553			AAGL
MOTA	2329		GLU		8.636			AAGL
MOTA .	2330		GLU		10.715			AAGL
MOTA	2331		PRO		11.893			AAGL
MOTA	2332							AAGL
MOTA	2333	CA	PRO	299	10.964	30.042 33.20-	, 1.00 21.70	

Fig. 3 cont.

122/174 37.913

AAGL 98.897 1.00 22.49 299 12.455 2334 CB PRO MOTA AAGL 98.826 1.00 23.37 36.429 2335 CG PRO 299 12.658 MOTA AAGL 10.133 38,131 97.924 1.00 21.34 299 2336 C PRO MOTA 1.00 25.08 AAGL 97.329 2337 39.203 O PRO 299 10.051 ATOM 97.507 AAGL 1.00 21.73 9.515 37.031 300 ALA 2338 N MOTA 1.00 23.94 AAGL 96.264 8.751 37.021 300 MOTA 2339 CA ALA 1.00 23.80 AAGL 9.418 36.071 95.272 2340 ALA 300 MOTA CB 36.663 96.386 1.00 23.97 AAGL 300 7.280 MOTA 2341 С ALA AAGL 1.00 24.57 .36.277 95.394 ALA 300 . 6.663 2342 0 MOTA AAGL 36.802 97.579 1.00 25.04 6.707 ATOM 2343 N TRP 301 1.00 24.04 AAGL 97.775 5.301 36.454 2344 CA TRP 301 MOTA AAGL 5.007 36.244 99.266 1.00 25.15 301 2345 TRP ATOM CB 1.00 23.59 AAGL 99.531 3.744 35.459 ATOM 2346 CG TRP 301 AAGL 34.781 100.744 1.00 23.73 3.394 2347 CD2 TRP 301 MOTA 34.200 100.54B 1.00 23.63 AAGL 2348 301 -2.119 CE2 TRP ATOM AAGL 34.607 101.980 1.00 24.03 CE3 TRP 301° 4.033 MOTA 2349 98.673. 1.00 23.60 AAGL 35.267 301 2.697 2350 CD1 TRP MOTA AAGL 1.00 24.88 1.717. 34.513 99.278 NEI TRP 301 MOTA 2351 1.00 22.63 AAGL 33.458 101.544 1.470 301 MOTA 2352 CZ2 TRP 1.00 22.92 AAGL 33,871 102.969 CZ3 TRP. 301 3.387 2353 **MOTA** AAGL 33.306 102.741 1.00 21.62 2.119 2354 CH2 TRP 301 ATOM 1.00 25.72 97.213 AAGL 301 4.322 37.485 2355 TRP ATOM C 3.682 AAGL 97.968 1.00 24.12 38.220 301 ATOM 2356 0 TRP AAGL 95.889 1.00 26.27 37.532 2357 N ILE 302 4.192 ATOM AAGL 1.00 26.33 95.256 3.273 38.475 ILE 302 ATOM 2358 CA 93.722 1.00 28.94 AAGL 3.257 38.317 302 2359 CB ILE ATOM 1.00 30.12 AAGL 39.615 93.081 CG2 ILE 302 2.804 MOTA 2360 93.215 1.00 32.05 AAGL 4.653 37.963 CG1 ILE 302 MOTA 2361 1.00 33.22 AAGL 5.671 39.038 93.462 302 CD1 ILE ATOM 2362 1.00 24.91 AAGL 95.770 2363 ILE 302 1.872 38.180 MOTA C 1.00 26.39 AAGL 1.467 · 37.017 95.B40 ILE 302 MOTA .0 2364 1.134 AAGL 39.223 96.133 1.00 25.25 2365 N GLY 303 MOTA 1.00 27.25 AAGL 96.646 303 -0.210 39.018 2366 CA GLY ATOM AAGL 39.086 98.159 1.00 26.83 -0.298 MOTA 2367 C GLY 303 AAGL 98.728 1.00 27.53 GLY 303 -1.39439.110 ATOM 2368 O AAGL 1.00 25.82 39.090 98.812 0.861 2369 ASN 304 ATOM N 1.00 23.80 AAGL 39.182 100.267 0.958 2370 CA ASN 304 MOTA AAGL 37.783 100.887 1.00 22.97 ASN 304 1.113 ATOM CB 2371 AAGL 1.00 23.62 37,811 102.413 ATOM 2372 CG ASN 304 1.131 1.00 25.26 AAGL 0.494 38.663 103.038 2373 OD1 ASN 304 MOTA 36.864 103.017 AAGL 1.00 20.66 304 1.841 ATOM 2374 ND2 ASN AAGL 1.00 22.75 304 2.200 40.031 100,539 2375 ASN ATOM C 39.704 101.382 1.00 21.47 AAGL 3.030 304 ASN MOTA 2376 0 AAGL 99.812 1.00 23.77 MOTA 2377 ALA 305 2.306 41.139 N AAGL ALA 3.454 3.281 42.028 99.926 1.00 23.13 305 MOTA 2378 CA 43.211 98,980 1.00 25.11 AAGL MOTA 2379 CB ALA 305 AAGL 1.00 22.70 305 3.770 42.520 101.335 2380 ALA С ATOM 1.00 23.39 AAGL 4.928 42.784 101.650 305 ATOM 2381 0 ALA 1.00 23.04 AAGL 42.632 102.182 GLY 306 2.753 MOTA 2382 М AAGL 43.093 103.543 1.00 21.61 2.970 306 MOTA 2383 CA GLY AAGL 1.00 20.83 42.023 104.421 2384 C GLY 306 3.592 MOTA AAGL 4.185 42.323 105.461 1.00 20.31 306 GLY MOTA 2385 0 AAGL 1.00 20.88 40.771 103.997 ATOM 2386 N LEU 307 3.445 AAGL 3.980 39.615 104.710 1.00 19.63 307 LEU ATOM 2387 CA 39.575 104.599 1.00 19.26 AAGL 5.511 LEU 307 MOTA 2388 CB AAGL 1.00 17.07 LEU 307 6.089 39.333 103.198 2389 CG ATOM 39.293 103.292 1.00 21.74 AAGL 7.602 CD1 · LEU 307 ATOM 2390 1.00 18.50 AAGL 5.568 38.012 102.625 CD2 LEU 307 MOTA 2391 1.00 20.69 1.00 20.75 3,580 39.543 106.178 AAGL 2392 LEU 307 ATOM C AAGL 4.377 39.131 107.018 2393 0 LEU 307 MOTA AAGL 2.352 39.955 106.484 1.00 19.76 2394 N GLY 308 ATOM 1.00 22.38 AAGL 39.898 107.854 1.870 MOTA 2395 CA GLY 308 AAGL 41.068 108.769 1.00 23.64 2.188 308 ATOM 2396 С GLY 1.00 23.65 AAGL 41.072 109.938 308 1.785 ATOM 2397 0 GLY AAGL 2,907 1.00 23.88 309 42.060 108.252 MOTA 2398 N SER AAGL 43.227 109.045 1.00 22.50 309 3.275 2399 CA. SER ATOM AAGL 43.684 108.695 1.00 22.00 4.693 CB SER 309 ATOM 2400

					<b>12</b>	3/174			
ATOM	2401	OG	SER	309	4.719	44.264	107.407	1.00 20.09	AAGL
ATOM	2402		SER	309	2.312	44.385	108.790	1.00 23.02 1.00 23.42	aagl aagl
MOTA	2403		SER	309	1.388	44.271	107.983	1.00 23.42	AAGL
MOTA	2404		SER	310	2.539	45.494 46.684	109.400	1.00 23.22	AAGL
ATOM	2405		SER	310	1.707 1.715	47.535	110.592	1.00 22.59	AAGL
MOTA	2406 2407		SER SER	310 310	3.022	48.003	110.903	1,00 24.03	AAGL
MOTA MOTA	2408	C	SER	310	2.234	47.512	108.138	1.00 23.44	AAGL
MOTA	2409	ŏ	SER	310	1.658	48.545	107.773	1.00 23.68	AAGL
ATOM	2410	N	CYS	311	3.340	47.069	107.548	1.00 21.68	AAGL
ATOM	2411	CA	CYS	311	3.892		106.413	1.00 23.63	AAGL
ATOM	2412	С	CYS	311	3.210		105.123	1.00 24.17 1.00 26.98	aagl aagl
MOTA	2413	0	CYS	311	2.591 5.387	46.321	105.044 106.289	1.00 25.30	AAGL
ATOM	2414	CB SG	CYS CYS	311 311	6.407	47.343	107.501	1.00 27.01	AAGL
MOTA MOTA	2415 2416	Ŋ	ALA	312	3.343		104.104	1.00 23.57	AAGL
ATOM	2417	CA	ALA	312	2.707			1.00 25.20	AAGL
MOTA	2418	СВ	ALA	312	2.516		102.053	1.00 25.76	AAGL
ATOM	2419	С	ALA	312	3.400		101.919	1.00 25.50	AAGL
ATOM	2420	0	ALA	312	2.741		101.288	1.00 24.61	AAGL AAGL
MOTA	2421	N	ASP	· 313	4.726		101.858	1.00 25.50 1.00 25.55	AAGL
ATOM	2422	CA	ASP	313	5.444 5.560	46.122	100.949 99.596	1.00 28.83	AAGL
MOTA	2423 2424	CB CG	ASP ASP	313 313	5.870	45.886	98.471	1.00 31.63	AAGL
ATOM · ATOM	2425		ASP	313	6.652	44.940	98.680	1.00 29.42	AAGL
MOTA	2426		ASP	313	5.337	46.107	97.358	1.00 37.09	AAGL
ATOM	2427	C		313	6.836		101.440	1.00 25.26	AAGL
ATOM	2428	0	ASP	313	7.698		101.575	1.00 25.34	AAGL
MOTA	2429	N	ASN	314		44.460	101.685 102.157	1,00 22.30 1.00 21.78	AAGL AAGL
MOTA	2430	CA	ASN	314	8.335 8.156		103.458	1.00 23.69	AAGL
MOTA	2431 2432	CB CG	asn Asn	314 314	7.832		104.640	1.00 25.29	AAGL
ATOM ATOM	2432		ASN	314	8.520		104.883	1.00 28.43	AAGL
ATOM	2434		ASN	314	6.787		105.382	1.00 24.92	AAGL
ATOM	2435	С	ASN	314	8.999		101.127	1.00 22.83	AAGL
ATOM	2436	0	ASN	314	10.043		101.393	1.00 21.72	aagl aagl
MOTA	2437	N	LEU	315	8.388	42.942		1.00 22.78 1.00 22.99	AAGL
ATOM	2438	CA	LEU	315 315	8.919 7.879	42.086 41.913		1.00 22.49	AAGL
ATOM ATOM	2439 2440	CB CG	LEU LEU	315	6.491	41.421	98.219	1.00 22.62	AAGL
ATOM	2441		LEU	315	5.599	41.214	96.991	1.00 25.48	AAGL
ATOM	2442		LEU	315	6.638	40.117	.98.978	1.00 23.90	AAGL
ATOM	2443	С	LEU	315	10.219	42.604		1.00 24.65	AAGL
MOTA	2444	0	LEU	315	10.608	43.756		1.00 24.23 1.00 25.62	AAGL AAGL
MOTA	2445	N	MET	316	10.898 12.135	41.728		1.00 28.28	AAGL
ATOM	2446 2447	CA CB	MET MET	316 316	13.280	41.159		1.00 26.81	AAGL
MOTA MOTA	2448	CG	MET	316	13.718	41.299	-	1.00 27.89	AAGL
ATOM	2449	SD	MET	316	15.182	40.302		1.00 29.46	AAGL
ATOM	2450	CE	MET	316	16.470	41.485		1.00 29.41	AAGL
MOTA	2451	С	MET	316	11.889	41.977		1.00 29.33	aagl aagl
ATOM	2452	0	MET	316	12.824	41.939 41.910		1.00 29.21 1.00 30.78	AAGL
MOTA	2453 2454	N	VAL VAL	317 317	10.616 10.217	41.820		1.00 30.70	AAGL
ATOM ATOM	2454	CA CB	VAL	317	9.681	40.416		1.00 31.88	AAGL
ATOM	2456		VAL	317	10.763	39.374		1.00 33.90	AAGL
ATOM	2457		VAL	317	8.479	40.100		1.00 36.43	AAGL
ATOM	2458	C	VAL	317	9.113	42.836			AAGL
MOTA	2459	0	VAL	317	8.342	43.169			AAGL AAGL
ATOM	2460	N	ASP	318	9.041	43.333			AAGL
ATOM	2461	CA	ASP	318	8.015 8.405	44.309			AAGL
MOTA	2462 2463	CB CG	ASP ASP	318 318	7.502	46.252			AAGL
MOTA MOTA	2463		ASP L ASP	318	6.267	46.066			AAGL
ATOM	2465		ASP	318	8.022	47.370			AAGL
ATOM	2466		ASP		6.671	43.621	L 91.547		AAGL
MOTA	2467		ASP	318	6.512	42.800	90.642	1.00 41.02	AAGL
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Fig. 3 cont.

					12	4/174			
ATOM	2468	N	TYR	319	5.695	43.985		1.00 43.91	AAGL
ATOM	2469		TYR	319	4.370	43.308	92.312	1.00 46.99	AAGL
MOTA	2470		TYR	319	3.555	43.811	93.548	1.00 48.59 1.00 48.66	aagl aagl
ATOM	2471		TYR	319	3.003	45.224 45.475	93.516 93.080	1.00 49.01	AAGL
ATOM	2472	CD1		319 319	1.702 1.180	46.778	93.066	1.00 49.49	AAGL
MOTA	2473 2474	CE1		319	3.772	46.305	93.937	1.00 49.12	AAGL
ATOM ATOM		· ČE2		319	3.264	47.610	93.929	1.00 49.13	. AAGL
MOTA	2476	CZ	TYR	319	1.967	47.836	93.493	1.00 49.15	AAGL
MOTA	2477	OH	TYR	319	1.457	49.115	93.495	1.00 48.83	AAGL AAGL
MOTA	2478	C	TYR	319	3.602 2.479	43.705	91.034 90.840	1.00 49.01 1.00 51.46	AAGL
MOTA	2479	0	TYR THR	319 320	4.178	43.221 44.522	90.158	1.00 48.98	AAGL
ATOM ATOM	2480 2481	N . ÇA	THR	320	3.491	44.827	88.909	1.00 48.98	AAGL
ATOM	2482	CB	THR	320	3.383	46.349	88.642	1.00 48.87	AAGL
ATOM	2483	OG1	THR	320	4.681	46.899	88.371	1.00 48.24	AAGL
ATOM	2484	CG2		320	2.770	47.054	89.829	1.00 48.99	aagl aagl
ATOM	2485	C	THR	320	4.206	44.184	87.730 86.896	1.00 49.75 1.00 50.61	AAGL
ATOM .	2486	N O	THR THR	320 321	3.572 5.524	43.536 44.349	87.671	1.00 49.77	AAGL
ATOM ATOM	2487 2488	CA	THR	321 .	6.316	43.798	86.575	1.00 50.22	· AAGL
ATOM	2489	CB	THR	321	7.561	44.673	86.297	1.00 50,80	AAGL
ATOM	2490.	OG1	THR	321	8.505	44.522	87.368	1.00 51.66	AAGL
ATOM	2491		THR	321	7.168	46.144	86.193	1.00 51.57	AAGL AAGL
MOTA	2492	C.	THR	321	6.805	42.371 41.743	86.807 85.905	1.00 50.77	AAGL
MOTA	2493 2494	O N	THR ASP	321 322	7.360 .6.617	41.743	88.016	1.00 49.25	AAGL
MOTA	2495	CA	ASP	322	7.082	40.515	88.345	1.00 47.20	AAGL
ATOM	2496	CB	ASP	322	6.534	39,471	87.354	1.00 50.64	AAGL
ATOM	2497	CG	ASP	322	5.010	39.462	87.262	1.00 52.01	AAGL
ATOM	2498		ASP	322	4.313	39.445	88.309	1.00 52.82 1.00 55.12	AAGL AAGL
ATOM	2499		ASP	322	4.502 8.616	39.442 40.486	86.113 88.288	1.00 44.47	AAGL
MOTA MOTA	2500 2501	С 0	asp asp	322 322	9.231	39.416	88.385	1.00 44.83	AAGL
ATOM	2502	N	GLU	323	9.236	41.652	88.124	1.00 41.39	AAGL
ATOM	2503	CA	GLU	323	10.696	41.745	88.049	1.00 39.30	AAGL
MOTA	2504	CB	GLU	323	11.093	42.894	87.127	1.00 41.31	AAGL
ATOM	2505	CG	GLU	323	12.586	43.108	86.977	1.00 44.75 1.00 47 ₋ 16	AAGL AAGL
ATOM	2506	CD	GLU GLU	323 323	12.911 14.099	44.040 44.371	85.812 85.612	1.00 47.71	AAGL
ATOM ATOM	2507 2508		GLU	323	11.971	44.438	85.091	1.00 47.99	AAGL
ATOM	2509	C	GLU	323	11.346	41.939	89.420	1.00 36.82	AAGL
ATOM	2510	0	ĠĿU	323	10.898	42.761	90.220	1.00 35.46	AAGL
ATOM	2511	N	VAL	324	12.410	41.182	89.675	1.00 35.31 1.00 32.93	AAGL AAGL
ATOM	2512	CA	VAL	324	13.120 14.154	41.257	90.948 91.099	1.00 32.93	AAGL
atom Atom	2513 2514	CB CG1	VAL VAL	324 324	13.487	38.770	90.827	1.00 32.75	AAGL
ATOM	2515		VAL	324	15.341	40.316		1.00 32.38	AAGL
ATOM	2516	С	VAL	324	13.864	42.573		1.00 33.56	AAGL
MOTA	2517	0	VAL	324	14.329	43.153		1.00 33.29	AAGL AAGL
MOTA	2518	N	TYR	325	13.974	43.045 44.282		1.00 30.85 1.00 31.59	AAGL
ATOM	2519	CA	TYR TYR	325 325	14.683 14.228	44.202		1.00 30.31	AAGL
MOTA MOTA	2520 2521	CB	TYR	325	12.794	45.387		1.00 31.58	AAGL
MOTA	2522		TYR	325	12.225	46.079		1.00 31.55	AAGL
MOTA	2523		TYR	325	10.908	46.548		1.00 33.68	AAGL
ATOM	2524	CD2	YYR	325	12.015				AAGL
ATOM	2525		TYR	325	10.714	45.639			AAGL AAGL
MOTA	2526 2527	CZ OH	TYR TYR	325 325	10.164 8.878	46.323 46.780		1.00 33.10	AAGL
atom Atom	2528	C	TYR	325 325	16.169			1.00 31.02	AAGL
ATOM	2529	õ	TYR	325	16.602			1.00 28.70	AAGL
ATOM	2530		GLU	326	16.946				AAGL
ATOM	2531	CA	GLU	326	18.398				AAGL AAGL
ATOM	2532		GLU	326	18.949				AAGL AAGL
ATOM	2533	CG	GLU GLU	326 326	20.432 20.851				AAGL
ATOM	2534	CD	GTO	220	20.631	41,554		2.00 .20	

Fig. 3 cont.

					12	5/174			
ATOM	2535	OE1	GLU	326	20.682	48.359	91.021	1.00 42.66	AAGL
ATOM	2536	OE2		326	21.334	48.731	93.106	1.00 40.82	AAGL
MOTA	2537	С	GLU	,326	18,848	44.538	94.065	1.00 29.10	AAGL
ATOM	2538	0	GLU	326	19.996	44.136	94.253	1.00 27.19	AAGL
MOTA	2539	Ν.	SER	327	17.939	44.581	95.035 96.387	1.00 27.41 1.00 25.31	AAGL AAGL
ATOM	2540	CA	SER	327	18.265	44.147 44.519	97.347	1.00 23.51	AAGL
ATOM	2541	CB	SER	327 327	17.127 15.870	44.218	96.776	1.00 25.25	AAGL
MOTA MOTA	2542 2543	OG C	SER SER	327	18.574	42.650	96.458	1.00 24.17	AAGL
ATOM	2544	Õ	SER	327	19.243	42.195	97.383	1.00 25.88	AAGL
ATOM	2545	N	ILE	328	18.107	41.880	95.479	1.00 27.45	AAGL
ATOM.	2546	CA	ILE	328	18.395	40.446	95.466	1.00 28.86	<b>AAGL</b>
MOTA	2547	CB	ILE	328	17.692	39.728	94.295	1.00 31.12	AAGL
ATOM	2548	CG2	ILE	328	18.120	38.277	94.250	1.00 35.58	AAGL
MOTA	2549	CG1		328	16.175	39.823	94.448	1.00 33.48	AAGL
MOTA	2550	CD1	•	.328	15.647	39.194	95.727	1.00 36.80 1.00 29.16	AAGL AAGL
MOTA	2551	C	ILE	328	19.904	40.248 39.324	95.317 95.897	1.00 27.50	AAGL
ATOM	2552	0	ILE	328 329 ·	20.486 20.536	41.124	94.538	1.00 30.01	AAGL
MOTA MOTA	2553 2554	N CA	GLU GLU	329	21.978	41.045	94.328	1.00 30.96	AAGL
ATOM	2555	СВ	GLU	329	22.435	42.017	93.229	1.00 33.99	AAGL
ATOM	2556	CG	GLU	329	21.773	41.813	91.866	1.00 37.96	AAGL
MOTA	2557	CD	GLU	329	22.520	42.542	90.746	1.00 42.17	AAGL
ATOM	2558	OE1	GLU	329	22.731	43.773	90.863	1.00 42.73	AAGL
MOTA	2559	OE2	GLŲ	329	22.898	41.883	89.746	1.00 42.99	AAGL
MOTA	2560	C.	GLU	329	, 22.682	41.386	95.627	1.00 29.64	AAGL
ATOM	2561	0	GLU	329	23.693	40.771	95.988 96.340	1.00 29.09 1.00 28.03	AAGL AAGL
ATOM	2562		THR	330	22.142 22.720	42.368 42.776	97.611	1.00 26.58	AAGL
MOTA	2563 2564	CA CB	THR THR	330 330	21.958	43.986	98.200	1.00 27.90	AAGL
ATOM ATOM	2565		THR	330	22.099	45.110	97.323	1.00 26.78	AAGL
ATOM	2566	CG2		330	22.495	44.345	99.574	1.00 27.91	AAGL
ATOM	2567	C	THR	330	22.671	41.608	98.606	1.00 26.92	AAGL
ATOM	2568	0	THR	330	23.654	41.325	99.301	1.00 25.31	AAGL
MOTA	2569	N	LEU	331	21.529	40.930	98.667	1.00 25.72	AAGL
· ATOM	2570	CA	LEU	331	21.368	39.791	99.571	1.00 24.97	AAGL AAGL
MOTA	2571	CB	LEU	331	19.923	39.282	99.532 100.247	1.00 24.19 1.00 23.31	AAGL
ATOM	2572	CG CD1	LEU	331 331	19.567 19.873		100.247	1.00 25.31	AAGL
ATOM ATOM	2573 · 2574		LEU	. 331	18.082	37.674	100.034	1.00 23.20	AAGL
ATOM	2575	C	LEU	331	22.319	38.674	99.158	1.00 25.90	AAGL
ATOM	2576	ō	LEU	331	22.971	38.054	100.001	1.00 25.54	AAGL
MOTA	2577	N	GLY	332	22.390	38.427	97.853	1.00 26.10	AAGL
ATOM	2578	CA	GLY	332	23.262	37.386	97.337	1.00 28.89	AAGL
ATOM	2579	С	GLY	332	24.738	37.631	97.594	1.00 31.12	AAGL AAGL
ATOM	2580	0	GLY	332	25.526	36.682	97.614 97.805	1.00 30.65 1.00 31.60	AAGL
ATOM	2581	N	GLU	333 333	25.120 26.524	38.890 39.229	98.044	1.00 31.00	AAGL
ATOM ATOM	2582 2583	CA CB	GLU	333	26.949	40.400	97.148	1.00 34.97	AAGL
ATOM	2584	CG	GLU	333	26.639	40.205	95.673	1.00 37.79	AAGL
ATOM	2585	CD	GLU	333	26.846	41.471	94.846	1.00 41.19	AAGL
ATOM	2586		GLU	333	26.164	41.621	93.807	1.00 40.67	AAGL
MOTA	2587	OE2	GLU	333	27.694	42.309	95.225	1.00 44.05	AAGL
ATOM	2588	C	GLU	333	26.844	39.586		1.00 35.01	AAGL
ATOM	2589	0	GLU	333	27.924	40.109	99.776	1.00 33.69	AAGL AAGL
ATOM	2590	N	LEU	334 334	25.925 26.193		100.410 101.805	1.00 34.35 1.00 33.87	AAGL
MOTA MOTA	2591 2592	CA CB	LEU LEU	334	24.963		102.672	1.00 33.01	AAGL
ATOM	2592	ÇG	LEU	334	23.721		102.407	1.00 32.82	AAGL
MOTA	2594		LEU	334	22.611		103.347	1.00 28.38	AAGL
ATOM	2595		LEU		24.044	41.711	102,607	1.00 30.26	AAGL
ATOM	2596	С	LEU		27.396		102.344	1.00 35.69	AAGL
ATOM	2597	0	LEU	334	27.475		102.129	1.00 36.26	AAGL
ATOM	2598	rxo	LEU	334	28.249	39.520	102.989	1.00 35.77	AAGL
END									

Fig. 3 cont.



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		•	12	6/174			PVS
HEADER					00.504	BLGL	BLGL
ATOM	1 C GLY	11		14.251	23.684 23.517	1.00 48.49 1.00 48.50	BĽGL
MOTA	2 O GLY	11	36.590	13.193 16.222	25.216	1.00 48.08	BLGL
ATOM	3 M GLY	11	36.372 36.733	15.548	23.933	1.00 47.57	BLGL
ATOM	4 CA GLY 5 N LEU	11 . 12	34.642	14.326	23.653	1.00 48.44	BLGL
MOTA MOTA	5 N LEU 6 CA LEU	12	33.796	13.147	23.416	1.00 45.49	BLGL
ATOM	7 CB LEU	12	32.592	13.139	24.371.	1.00 43.64	BLGL
ATOM	8 CG LEU	12	31.626	11.961	24.199	1.00 41.45	BLGL
ATOM	9 CD1 LEU	12	32.074	10.803	25.085	1.00 36.51	BLGL
MOTA	10 CD2 LEU	12	30.203	12.400	24.550	1.00 41.11	BLGL BLGL
MOTA	11 C LEU	12	33.272	13.109 14.086	21.979 21.502	1.00 44.11	BLGL
ATOM	12 O LEU	12 :	32.688 33.487	11.986	21.295	1.00 42.63	BLGL
MOTA	13 N TYR 14 CA TYR	13 13	33.004	11.817	19.928	1.00 41.19	BLGL
ATOM ATOM	14 CA TYR 15 CB TYR	13 -	34.083	11.206	19.042	1.00 45.36	BLGL
ATOM	16 CG TYR	13	33.594	10.996	17.624	1.00 52.03	BLGL
ATOM	17 CD1 TYR	13	33.232	9.727	17.167	1.00 53.91	BLGL
ATOM	18 CEL TYR	13	32.703	9.545	15.872	1.00 55.69	BLGL
MOTA	19 CD2 TYR	13	33.420	12:083	16.756	1.00 53.77 1.00 54.66	BLGL . BLGL
MOTA	20 CE2 TYR	13	32.890 32.534	11.914 10.644	15.466 15.031	1.00 56.09	BLGL
ATOM	21 CZ TYR	13 13	32.534	10.473	13.764		BLGL
ATOM	22 OH TYR 23 C TYR	13	31.755	10.932	19.837	1.00 38.22	BLGL
ATOM ATOM	24 O TYR	13	31.686	9.887	20.471	1.00 38.74	BLGL
ATOM	25 N .VAL	14	30.776	11.355	19.039	1.00 34.88	BLGL
MOTA	26 CA VAL	14	29.537	10.604	18.845	1.00 31.50	BLGL
ATOM	27 CB VAL	14	28.418	11.094	19.777	1.00 30.78	BLGL BLGL
ATOM	28 CG1 VAL	14	27.102	10.405	19.427 21.203	1.00 30.71 1.00 30.70	BLGL
MOTA	29 CG2 VAL	14	28.790 29.069	10.812 10.798	17.420	1.00 30.74	BLGL
MOTA	30 C VAL 31 O VAL	14 14	28.776	11.917	17.007	1.00 31.52	BLGL
ATOM ATOM	32 N GLU	15	28.994	9.710	16.669	1.00 30.21	BLGL
ATOM	33 CA GLU	15	28.555	9.788	15.288	1.00 30.31	BLGL
ATOM	34 CB GLU	15	29.002	8.546	14.534	1.00 33.96	BLGL
ATOM	35 CG GLU	15	28.509	8.486	13.113	1.00 43.05	BLGL BLGL
ATOM	36 CD GLU	15	28.927	7.202	12.424	1.00 49.32 1.00 51.29	BLGL
MOTA	37 OE1 GLU	15	28.886 29.285	6.140 7.251	13.087 11.223	1.00 54.28	BLGL
ATOM	38 OE2 GLU 39 C GLU	15 15	27.045	9.931	15.206	1.00 28.83	BLGL
ATOM ATOM	40 O GLU	15	26.303	9.161		1.00 26.88	BLGL
ATOM	41 N LYS	16	26.596	10.923		1.00 29.24	BLGL
ATOM	42 CA LYS	16	25.173	11.173		1.00 30.57	BLGL
MOTA	43 CB LYS	16	24.933	12.207		1.00 32.52	BLGL BLGL
ATOM	44 CG LYS	16	23.454	12.496		1.00 38.94	BLGL
ATOM	45 CD LYS	16	23.141 23.632	12.889 14.282		1.00 46.85	BLGL
MOTA	46 CE LYS 47 NZ LYS	16 16	23.276	14.648			BLGL
MOTA MOTA	48 C LYS	16	24.399	9.902			BLGL
ATOM	49 O LYS	16	24.836	9.090		1.00 28.75	
ATOM	50 N VAL	17	23.249	9.733			
MOTA	51 CA VAL	17	22.394	8.591			
MOTA	52 CB VAL	17	21.437	8.328 7.201			
ATOM	53 CG1 VAL	17 17	20.469 22.236	7.982			
ATOM ATOM	54 CG2 VAL 55 C VAL	17	21.582	8.940			
ATOM	56 O VAL	17	20.794	9.891		1.00 30.98	
ATOM	57 N SER	18	21.782	8.172			
MOTA	58 CA SER	18	21.083	8.422			
ATOM	59 CB SER	18	21.787	7.675			
MOTA	60 OG SER	18	21.984	б.324			
MOTA	61 C SER	18	19.611	8.032 6.933			
ATOM	62 O SER	18	19.264 18.755				
MOTA	63 N GLY 64 CA GLY	19 19	17.328				
MOTA MOTA	65 C GLY	19	16.601				
22 WE					_		

Fig. 4

			40	~ 14 7 4		PVS	}
		•	12	7/174			77.01
ATOM	66 O GLY	19	15.395	8.684	11.705	1.00 32.49 1.00 28.46	Blgl Blgl
MOTA	67 N LEU	20	17.314	9.295	12.681 13.967	1.00 28.48	BLGL
MOTA	68 CA LEU	20	16.672	9.498 9.910	15.013	1.00 20.20	BLGL
MOTA	69 CB LEU	20	17.706	9,910	16.436	1.00 29.10	BLGL
MOTA	70 CG LEU	20 20	17.141 16.756	8.586	16.904	1.00 27.36	BLGL
MOTA	71 CD1 LEU 72 CD2 LEU	20	18.165	10.598	17.359	1.00 29.58	BLGL
MOTA MOTA	72 CD2 LEU 73 C LEU	20	15.565	10.548	13.890	1.00 25.87	BLGL
MOTA	74 O LEU	20	15.821	11.686	13.535	1.00 24.28	BLGL
ATOM	75 N ARG	21	14.342	10.147	14.226	1.00 28.07	BLGL
MOTA	76 CA ARG	21	13.176	11.030	14.213	1.00 30.64	BLGL
MOTA	77 CB ARG	21	11.912	10.211	14.476	1.00 31.64 1.00 35.81	BLGL BLGL
ATOM	78 CG ARG	21	11.955	9.430	15.792 15.840	1.00 35.81	BLGL
MOTA	79 CD ARG	21	10.892 9.536	8.339 8.877	15.850	1.00 37.50	BLGL
MOTA	80 NE ARG	21 21	8.445	8.133	15.699	1.00 38.47	BLGL
MOTA	81 CZ ARG 82 NH1 ARG	21	8.567	6.826	15.525	1.00 37.04	BLGL
MOTA MOTA	83 NH2 ARG	21	7.235	B.688	15.731	1.00 39.56	Brer .
ATOM	84 C ARG	21	13.316	12,114	15.277	1.00 32.05	BLGL
· ATOM	85 O ARG	21	13.840	11.862	16.354	1.00 31.41	BLGL
ATOM	86 N LYS	22	12.832	13.315	14.978	1.00 35.57	BLGL
ATOM	87 CA LYS	22	12.927	14.428	15.916	1.00 37.84	BLGL BLGL
ATOM	88 CB LYS	22	12.378	15.713	15.291	1.00 42.04 1.00 47.84	BLGL
ATOM	89 CG LYS	22	13.278	16.381 17.872	14.265 14.150	1.00 47.84	BLGL
MOTA	90 CD LYS	22 22	12.908 13.460	18.518	12.882	1.00 52.80	BLGL
ATOM	91 CE LYS 92 NZ LYS	22	12.732	18.062	11.661	1.00 52.64	BLGL
MOTA MOTA	92 NZ LYS 93 C LYS	22	12.225.	14.227	17.253	1.00 36.42	BLGL
ATOM	94 O LYS	22	12.672	14.762	18.264	1.00 37.54	BLGL
ATOM	95 N ASP	. 23	11.128	13.476	17.262	1.00 34.94	BLGL
ATOM	96 CA ASP	23	10.370	13.264	18.495	1.00 33.91	BLGL
ATOM '	97 CB ASP	23	8.869	13.257	18.181	1.00 34.54	BLGL BLGL
ATOM	98 CG ASP	23	8.465	12.096	17.303	1.00 34.79 1.00 33.67	BLGL
ATOM	99 OD1 ASP	23	9.242	11.739 11.547	16.392 17.521	1.00 33.67	BLGL
ATOM	100 OD2 ASP	23 23	7.365 10.754	11.989	19.238	1.00 31.78	BLGL
ATOM ATOM	101 C ASP 102 O ASP	23	10.001	11.495	20.083	1.00 31.40	BLGL
ATOM	102 O RSF	24	11.932	11.467	18.921	1.00 28.21	BLGL
ATOM	104 CA PHE	24	12.423	10.256	19.551	1.00 25.65	BLGL
ATOM	105 CB PHE	24	13.788	9.904	18.967	1.00 25.73	BLGL
ATOM	106 CG PHE	24	14.281	8.538	19.337	1.00 25.81	BLGL BLGL
ATOM	107 CD1 PHE	24	15.134	8.359	20.422	1.00 25.77 1.00 25.98	Brer
MOTA	108 CD2 PHE	24	13.930	7.431 7.093	18.573 20.739	1.00 25.74	BLGL
ATOM	109 CE1 PHE	24 24	15.642 14.431	6.161	18.881	1.00 27.08	BLGL
ATOM	110 CE2 PHE	24	15.292	5.992			BLGL
ATOM ATOM	111 C2 PHE 112 C PHE	24	12.517	10.473			BLGL
MOTA	113 O PHE	24	12.961	11.520	21.519	1.00 23.30	BLGL
ATOM	114 N ILE	25	12.077	9.474			BLGL
ATOM	115 CA ILE	25	12.096	9.514			BLGL BLGL
MOTA	116 CB ILE	25	11.137	8.465			BLGL
MOTA	117 CG2 ILE	25	11.388	8.253 8.883			· BLGL
ATOM	118 CG1 ILE	25	9.706 8.696	7.834			BLGL
MOTA	119 CD1 ILE 120 C ILE	25 25	13.487	9.227			BLGL
MOTA MOTA	120 C ILE	25 25	14.091	8.211		1.00 16.53	BLGL
MOTA	122 N LYS	26	13.985	10.128		1.00 16.78	BLGL
ATOM	123 CA LYS	26	15.294	9.962			BLGL
ATOM	124 CB LYS	26	16.213	11.096		1.00 19.07	BLGL
MOTA	125 CG LYS	26	16.276				BLGL
ATOM	126 CD LYS	26	16.943				BLGL BLGL
ATOM	127 CE LYS	26	16.949				BLGL
ATOM	128 NZ LYS	26 26	17.505 15.032				BLGL
ATOM	129 C LYS 130 O LYS	26 26	14.990				BLGL
ATOM ATOM	130 O LYS 131 N GLY	20 27	14.845				BLGL
21.00	"			4	4		

Fig. 4 cont.

128/174 BLGL 8.822 28.783 1.00 14.87 27 14.540 132 CA GLY ATOM BLGL 29.706 1.00 15.36 15.553 8.183 27 MOTA 133 С GLY BLGL 7.523 29.278 1:00 14.26 16.490 27 134 0 GLY MOTA BLGL 1.00 15.73 30.997 15.364 8.413 28 135 N VAL ATOM BLGL 7.847 32.002 1.00 15.81 16.233 136 CA VAL 28 ATOM 1.00 15.33 BLGL 32.505 17.285 8.866 28 137 CB VAL ATOM BLGL 31.359 1.00 15.90 18.189 9.289 28 CG1 VAL 138 MOTA 1.00 15.60 BLGL 33.113 10.073 16.604 139 CG2 VAL 28 MOTA BLGL 1.00 17.23 7.411 33.164 15.367 28 VAL 140 С MOTA 1.00 16.45 BLGL 33.405 14.294 7.967 28 141 0 VAL ATOM BLGL 1.00 17.41 33.860 15.817 6.380 N ASP 29 ATOM 142 1.00 18.06 BLGL 5.902 35.023 15.098 29 CA ASP MOTA 143 BLGL 1.00 16.28 14.855 4.391 34.925 ASP 29 MOTA 144 CB BLGL 1.00 18.27 3.832 36.138 29 14.123 145 CG ASP ATOM BLGL 1.00 15.84 35.978 13.426 2.801 29 ODI ASP MOTA 146 1.00 14.09 BLGL 4.409 37.246 14.258 147 QD2 ASP 29 MOTA 1.00 17.72 BLGL 36.201 6.248 ASP 29 16.006 148 C MOTA 1.00 18.18 BLGL 36.362 17.075 5.670 ASP 29 MOTA 149 0 BLGL 1.00 17.06 36.994 15.592 7.228 VAL 30 150 N MOTA 1.00 14.73 BLGL 7.653 38.158 16.360 ATOM 151 CA VAL 30 BLGL 1.00 13.70 38.051 9.151 16.740 VAL 30 152 CB MOTA 1.00 12.16 BLGL 17.688 9.354 36.880 30 ATOM 153 CG1 VAL BLGL 1.00 9.08 37.872 10.017 CG2 VAL 30 15.485 154 MOTA 1.00 14.73 BLGL 7.422 39.426 15.551 30 MOTA 155 C VAL BLGL 40.302 1.00 16.61 8.275 15.491 0. VAL 30 156 MOTA 1.00 16.05 BLGL 14.931 6.252 39.515 31 SER 157 N MOTA 5.899 1.00 19.01 BLGL 40.660 14.090 CA SER 31 ATOM 158 40.481 - 1.00 17.38 BLGL 13.540 4.481 31 159 CB SER MOTA BLGL 39.331 1.00 19.20 4.395 12.719 160 OG SER 31 MOTA 1.00 19.31 BLGL 42.030 SER 14.769 6.007 31 MOTA 161 С BLGL 6.282 43.041 1.00 19.82 14.120 SER 31 ATOM 162 0 42.059 BLGL 1.00 18.54 32 16.075 5.797 SER MOTA 163 N BLGL 1.00 19.36 16.826 5.845 43.301 SER 32 АТОМ 164 CA BLGL 1.00 18.42 43.133 18.121 5.055 SER 32 165 CB ATOM BLGL 1.00 16.54 5.611 42.088 18.909 SER 32 MOTA 166 OG 43.775 1.00 21.13 BLGL 7.259 17.161 32 ATOM 167 Ç SER BLGL 44.902 1.00 20.54 17.612 7.442 32 168 0 SER ATOM 1.00 21.96 BLGL 42.925 8.256 33 16.931 169 N ILE MOTA BLGL 1.00 22.33 43.263 17.256 9.644 ATOM 170 CA ILE 33 42.161 1.00 21.13 BLGL 16.752 10.622 33 171 CB ILE MOTA BLGL 1.00 19.56 42.095 15.234 10.621 172 CG2 ILE 33 MOTA BLGL 42.439 1.00 20.03 CG1 ILE 17.283 12.027 33 MOTA 173 BLGL 1.00 17.45 42.425 18.794 12.117 ILE 33 MOTA 174 CD1 1.00 23.71 BLGL 44.636 16.796 10.152 33 175 ILE MOTA C BLGL 1.00 25.43 10.858 45.309 17.549 MOTA 176 Ó ILE 33 1.00 24.35 BLGL 9.797 45.059 15.581 ILE 34 MOTA 177 N 1.00 23.98 BLGL 10.235 46.362 15.066 178 CA ILE 34 MOTA BLGL 46.486 1.00 23.20 9.951 13.539 179 CB ILE 34 ATOM 1.00 24.75 BLGL 9.637 47.922 13.170 180 CG2 ILE 34 MOTA BLGL 46.063 1.00 20.84 12.735 11.183 CG1 ILE 34 181 MOTA BLGL 1.00 21.81 13.078 11.696 44.729 MOTA 182 CD1 ILE 34 1.00 24.38 BLGL 9.598 47.550 15.815 34 ILE 183 C MOTA BLGL 1.00 25.31 16.186 10.290 48.502 MOTA 184 0 ILE 34 BLGL 1.00 22.66 47.500 16.041 8.290 N ALA 35 ATOM 185 1.00 22.83 BLGL 7.622 48.579 16.761 35 ATOM 186 CA ALA 1.00 20.64 BLGL 6.117 48.344 CB ALA 35 16.803 187 MOTA 1.00 23.42 BLGL 48.681 18.178 8.165 MOTA 188 C ALA 35 1.00 25.98 BLGL 49.776 8.377 189 ALA 35 18.687 0 ATOM 1.00 23.28 BLGL 18.813 8.382 47.536 36 190 И LEU MOTA 47.508 1.00 25.90 BLGL 8.900 191 CA LEU 36 20.173 ATOM BLGL 1.00 26.42 20.726 8.908 46.073 192 CB LEU 36 MOTA BLGL 45.421 1.00 25.94 21.093 7.671 CG LEU 36 193 MOTA BLGL 1.00 29.58 21.783 7,836 44.105 194 CDI LEU 36 MOTA 1.00 28.67 BLGL 46.323 22.017 6.778 195 CD2 LEU 36 MOTA BLGL 1.00 26.59 20.237 10.308 48.089 LEU 36 MOTA 196 C BLGL 1.00 25.84 21.140 10.637 48.863 197 Ω LEU MOTA

Fig. 4 cont.

					12	9/174			•
ATOM	i98	N	GLU	37	19.282	11.144	47.708	1.00 26.12	BLGL
MOTA	199		GLU	37	19.259	12.501	48.214	1.00 28.35	BLGL
ATOM	- 200		GLU	37	18.092	13.264	47.594	1.00 26.08	BLGL
MOTA	201		GLU	37	18.409	13.814	46.220	1.00 29.12	BLGL
MOTA	202		GLU	37	17.238	14.542	45.612	1.00 30.50 1.00 26.60	BLGL BLGL
MOTA	203	OE1		3.7	17.422	15.243	44.593 46.163	1.00 25.60	BLGL
MOTA	204		GLU	37	16.128 19.170	14.400 12.526	49.739	1.00 28.90	BLGL
MOTA	205		GLU GLU	37 37	19.828	13.334	50.393	1.00 30.03	BLGL
ATOM ATOM	206 207	O N	GLU	38	18.366	11.633	50.301	1.00 29.70	BLGL
MOTA	208		GLU	38	18.212	11.570	51.746	1.00 31.72	BLGL
ATOM	209	СВ	GLU	38	17.037	10.677	52.125	1.00 31.95	ŖLGL
ATOM	210	CG	GĽU	38	15.752	11.052	51.450	1.00 37.83	BLGL
MOTA	211	CD	GLU	38	14.562	10.379	52.094	1.00 40.58	BLGL BLGL
MOTA	212	OE1		38 .	-14.609	9.150	52.302 52.390	1.00 39.84 1.00 45.75	BLGL
ATOM	213	OE2		38	13.578 19.467	11.086 11.026		1.00 32.56	BLGL.
MOTA	214	С 0	GLU GLU	38 38	19.441	11.156	53.627	1.00 36.26	BLGL
ATOM ATOM	215 216	N.	SER	39	20.335	10.402	51.632	1.00 30.07	BLGL
ATOM	217	CA	SER	39	21.553	9.842	52.176	1.00 27.49	BLGL
ATOM	218	СВ	SER	39	21.939	8.602	51.379	1.00 29.09	BLGL
ATOM	219	OG	SER	39	20.872	7.667	51.376	1.00 24.83	BLGL
MOTA	220	C	SER	39	22.660	10.882	52.133	1.00 28.20	BLGL
ATOM	221	Ο.	SER	39	23.791	10.624	52.547	1.00 29.82 1.00 28.31	BLGL BLGL
ATOM .	222	N	GLY	40	22.327 23.303	12.063 13.135	51.626 51.558	1.00 20.31	BLGL .
MOTA	223	CA.	GLY	40 40	23.303	13.332	50.214	1.00 29.65	BLGL
at'om atom	225	Ö	GLY	40		14.296	50.031	1.00 31.52	BLGL
ATOM	226	N	VAL	41	23.730	12.428	49.272	1.00 28.2 <del>9</del>	BLGL
ATOM	227	CA	VAL	41	24.333	12.540	47.948	1.00 27.33	BLGL
MOTA	228	СВ	VAL	41	24.014	11.299	47.075	1.00 26.80	BLGL.
ATOM	229		VAL	41	24.634	11.458	45.699	1.00 24.11 1.00 25.53	BLGL BLGL
MOTA	230		VAL	41	24.531 23.816	10.034 13.788	47.754 47.242	1.00 23.53	BLGL
MOTA MOTA	231 232	C O	VAL VAL	41 41	22.630	14.107	47.315	1.00 27.71	BLGL
ATOM	233	N	ALA	42	24.716	14.496	46.568	1.00 28.05	$\mathtt{BLGL}$
MOTA	234	CA	ALA	42	24.364	15.713	45.840	1.00 27.62	BLGL
MOTA	235	CB	ALA	42	24.952	16.935	46.538	1.00 26.85	BLGL
ATOM	236	С	ALA	42	24.898	15.624	44.415	1.00 28.00 1.00 29.09	BLGL BLGL
MOTA	237	0	ALA	42 43	25.918	14.986 -16.267	43.489	1.00 27.56	BLGL
ATOM ATOM	238 239	N CA	PHE PHE	43	24.625	16.244	42.101	1.00 30.30	BLGL
MOTA	240	CB	PHE	43	23.529	15.626	41.223	1.00 29.43	BLGL
ATOM	241	CG	PHE	43	23.281	14.176	41.513	1.00 29.78	BLGL
MOTA	242	CD1	PHE	43	22.538	13.791	42.630	1.00 26.96	BLGL
MOTA	243		PHE	43	23.855	13.188	40.714	1.00 28.78 1.00 25.96	BLGL BLGL
MOTA	244		PHE	43	22.373	12.442 11.835	42.957 41.031	1.00 28.67	BLGL
ATOM	245		PHE	43 43	23.698	11.461	42.160	1.00 26.33	BLGL
MOTA MOTA	246 247	CZ C	PHE	43	24.954	17.651	41.632	1.00 32.38	BLGL
ATOM	248	Ö	PHE	43	24.351	18.622	42.096	1.00 33.12	BLGL
ATOM	249	N	TYR	44	25.915	17.759	40.719	1.00 32.89	BLGL
MOTA	250	CA	TYR	44	26.326	19.054	40.203	1.00 34.23	BLGL
MOTA	251	CB	TYR	44	27.807	19.289	40.482 41.926	1.00 33.04 1.00 33.71	BLGL BLGL
ATOM	252		TYR	44 44	28.165 28.177	19.083			BLGL
ATOM	253 254		L TYR L TYR	44	28.453				BLGL
ATOM ATOM	254 255		TYR	44	28.444			1.00 34.36	BLGL
ATOM	256		TYR	44	28,721			1.00 34.85	BLGL
ATOM	257		TYR	44	28.722		44.627		BLGL
ATOM	258	OH	TYR	44	28.974			1.00 37.37	BLGL
ATOM	259		TYR	4.4	26.085				BLGL BLGL
ATOM	260		TYR		25.531				BLGL
MOTA	261 262		ASN ASN	45 45	26.509 26.350				BLGL
ATOM ATOM	262 263		ASN	45	25.429				BLGL
				the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the s					

Fig. 4 cont.

						UILIT			
ATOM	264	CG	ASN	45	26.156	22.912	36.452	1.00 47.10 1.00 44.32	BLGL BLGL
ATOM	265	OD1		45	26.932 25.897	23.180 23.760	37.373 35.464	1.00 49.84	BLGL
MOTA	266	ND2 C	ASN ASN	45 45	27.721	20.618	36.038	1.00 43.53	BLGL
ATOM ATOM	267 268	ò	ASN	45	28.746	20.564	36.718	1.00 41.75	BLGL
ATOM	269	N	GLU	46	27.733	20.861	34.735	1.00 47.02	BLGL
ATOM	270	CA	GLU	46	28.979	21.090	34.011	1.00 51.61	BLGL
ATOM	271	CB	GLU	46	28.673	21.715	32.656	1.00 55.53	BLGL BLGL
ATOM	272	CG	GLU	46	27.635	20.976	31.820 31.261	1.00 59.75 1.00 62.26	BLGL
ATOM	273	CD	GLU	46 46	28.162 29.304	19.673 19.665	30.749	1.00 62.20	BLGL
ATOM	274 275		GLU GLU	46	27.429	18.665	31.320	1.00 63.83	BLGL
MOTA ATOM	276	C	GTO	46	29.917	22.027	34.782	1.00 52.77	BLGL
ATOM	277	Õ.	GLU	46	31.035	21.648	35.144	1.00 52.27	BLGL
ATOM	278	N	SER	47 .	29.440	23.248	35.029	1.00 53.78	BLGL
MOTA	279	CA	SER	47	30.197	24.288	35.723	1.00 54.29	· BLGL BLGL
ATOM	280	CB	SER	47 ·	29.312	25.518	35.940 34.707	1.00 56.24 1.00 57.54	BLGL
ATOM	281	og	SER	47 47	28.822 30.779	26.029 23.857	37.058	1.00 54.34	BLGL
ATOM ATOM	282 283	С 0	SER SER	47	31.720	24.477	37.552	1.00 56.28	BLGL
ATOM	284	N	GLY	48	30.215	_	37.651	1.00 53.12	BLGL
ATOM	285	CA	GLY	48	30.724	22.344	38.926	1.00 52.44	BLGL
ATOM	286	С	GLY.	48 .	29.883	22.783	40.109	1.00 52.32	BLGL BLGL
MOTA	287	0	GLY	48	30.200	22.455	41.258	1.00 51.88 . 1.00 51.68	BLGL
ATOM '	288	N.	LYS	49	28.807 27.919	23.518 24.009	39.832 40.882	1.00 50.92	BLGL
MOTA MOTA	289 290	CA CB	LYS LYS	49 49	27.338	25.368	40.477	1.00 52.51	BLGL
ATOM	291	,CG	LYS	49	26.440	25.314	39.255	1.00 54.74	BLGL
MOTA	292	CD	LYS	49	26.139	26.704	38.706	1.00 58.30	BLGL
ATOM	293	CE	LYS	.49	25.326	27.551	39.672	1.00 59.50	BLGL
ATOM	294	NZ	LYS	49	25.039	28.909	39,112	1.00 61.13 1.00 49.26	BLGL BLGL
MOTA	295	C	LYS	49	26.779 26.215	23.039 22.391	41.204	1.00 49.20	BLGL
MOTA	296 297	O N	LYS LYS	49 50	26.213	22.953	42.483	1.00 46.67	BLGL
ATOM ATOM	298	CA	LYS	50	25.377	22.082	42.955	1.00 44.89	BLGL
ATOM	299	CB	LYS	50	25.229	22.272	44.465	1.00 44.47	BLGL
ATOM	300	CG	LYS	50	24.483	21.182	45.190	1.00 47.37	BLGL
ATÓM	301	CD	LYS	50	24.732	21.290	46.692	1.00 50.81 1.00 53.40	BLGL BLGL
ATOM	302	CE	LYS	50	23.926 24.326	20.260	47.478 48.917	1.00 55.24	BLGL
ATOM ATOM	303 304	NZ C	LYS LYS	50 50	24.320	22.473	42.221	1.00 43.33	BLGL
MOTA	305	ō	LYS	50	23.726	23.647	42.187	1.00 43.90	BLGL
ATOM	306	Ŋ	GLN	51	23.400	21.497	41.631	1.00 41.68	BLGL
ATOM	307	CA	GLN	51	22.167	21.765	40.884	1.00 38.41	BLGL
MOTA	308	CB	GLN	51	22.531	22.164	39.449	1.00 38.23 1.00 38.66	BLGL BLGL
ATOM	309	CG	GLN	51	21.352 21.797	22.358 22.731	38.507 37.099	1.00 38.67	BLGL
ATOM ATOM	310 311	CD CD	GLN GLN	51 51	22.206	23.862	36.846	1.00 38.64	BLGL
ATOM	312		2 GLN	51	21.730	21.771		1.00 38.86	BLGL
ATOM	313	C	GLN	51	21.241	20.548	40.867	1.00 35.96	BLGL
MOTA	314	0	GLN	51	21.714	19.417	40.893	1.00 35.98	BLGL
ATOM	315	N	ASP	52	19.928	20.778	40.827	1.00 34.78 1.00 34.16	BLGL BLGL
MOTA	316	CA		52	18.955 17.522	19.677 20.215	40.797 40.657	1.00 35.75	BLGL
ATOM	317 318	CB CG	ASP ASP	52 52	16.475			1.00 36.25	BLGL
atom atom	319		1 ASP	52	15.271	19.396		1.00 35.18	BLGL
ATOM	320		2 ASP	52	16.857			1.00 41.59	BLGL
MOTA	321	C	ASP	52	19.269				BLGL
ATOM	322	0	ASP	52	19.475			1.00 33.59	BLGL
ATOM	323	N	ILE	53	19.294				BLGL BLGL
ATOM	324	CA		53 53	19.620 19.692				BLGL
ATOM ATOM	325 326		ILE 2 ILE	53 53	18.304				BLGL
ATOM	327		1 ILE	53	20.326			1.00 25.86	BLGL
ATOM	328		1 ILE	53	20.638			1.00 25.81	BLGL
MOTA	329		ILE	53	18.644	16.588	37.631	1.00 25.41	BLGL

Fig. 4 cont.

					4.4	11117			
ATOM	330	0	ILE	53	19.042		36.475	1.00 23.70 1.00 23.59	BLGL BLGL
ATOM	331	N	PHE	54	17.372	16.836 16.930	37.926 36.868	1.00 25.83	BLGL
MOTA	332 333	CA CB	PHE	54 54	16.380 14.972	17.002	37.456	1.00 23.83	BLGL
atom Atom	334	CG	PHE	54	14.526	15.723	38.072	1.00 22.74	BLGL
ATOM	335	CD1		54	14.799	15.449	39.402	1.00 25.01	BLGL
MOTA	336	CD2		54	13.885	14.760	37.306	1.00 21.32	Brcr
ATOM	337	CEl	PHE	54	14.443	14.229	39.961	1.00 27.14	BLGL
ATOM	338	CE2	PHE	54	13.525	13.537	37.856	1.00 23.72	BLGL BLGL
MOTA	339	CZ	PHE	54	13.803	13.268	39.184 35.953	1.00 24.12 1.00 27.75	BLGL
ATOM	340	C	PHE	54	16.641 16.378	18.121 18.064	34.753	1.00 27.75	BLGL
ATOM	341 342	O N	PHE ASN	54 55	17.167	19.197	36.522	1.00 30.60	BLGL
MOTA MOTA	343	CA	ASN	55 ·	17.485	20.385	35.740	1.00 32.40	BLGL
ATOM	344	CB	ASN	55	17.927	21.528	36.665	1.00 38.72	BLGL
MOTA	345	CG	ASN	55	18.157	22.835	35.919	1.00 43.16	BLGL
ATOM	34.6		ASN	55	18.775	23.767	36.444	1.00 46.30	BLGL
MOTA	347	•	ASN	55	17.657	22.912	34.692	1.00 47.38 1.00 30.86	BLGL BLGL
ATOM	348	Ç	ASN	55	18.631	19.996 20.327	34.808 33.623	1.00 30.30	BLGL
ATOM	349	0	asn Thr	55 56	18.624 19.608	19.281	35.363	1.00 28.42	BLGL
MOTA MOTA	350 351	n Ca	THR	56	20.765	18.824	34.606	1.00 26.82	BLGL
ATOM	352	CB	THR	56	21.769	18.101	35.514	1.00 27.58	BLGL
ATOM	353		THR	56	22.198	18.988	36.558	1.00 29.47	BLGL
ATOM	354	CG2	THR	56	22.969	17.642	34.714	1.00 22.45	BLGL
MOTA	355	С	THR	56	20.353	17.870	33.489	1.00 27.22	BLGL
MOTA	356	0	THR	56	20.851	17.952 16.961	32.366 33.805	1.00 27.23 1.00 27.52	BLGL
MOTA	357	N N	Leu Leu	57 57	19.441 18.950	15.997	32.830	1.00 27.32	BLGL
ATOM ATOM	358 359	CA CB	LEU	57	17.978	15.033	33.508	1.00 26.87	BLGL
MOTA	360	CG	LEU	57	18.453	13.617	33.847	1.00 26.41	BLGL
ATOM	361		LEU	57	19.941	13.572	34.078	1.00 23.65	BLGL
ATOM	362	CD2	LEU	57	17.691	13,138	35.074	1.00 25.32	BLGL
ATOM	363	С	LEU	57	18.257	16.686	31.662	1.00 28.88	BLGL BLGL
MOTA	364	0	LEU	57	18.430	16.288 17.718	30.515 31.959	1.00 29.93 1.00 30.47	BLGL
MOTA	365	N CA	LYS LYS	58 58	17.474 16.757	18.455	30.926	1.00 30.56	BLGL
ATOM ATOM	366 367	CB	LYS	58	15.836	19.507	31.561	1.00 32.82	BLGL
ATOM	368	CG		. 58	15.038	20.330	30.551	1.00 33.72	BLGL
ATOM	369	CD	LYS	58	14.129	19.438	29.710	1.00 36.45	BLGL
MOTA	370	CE	LYS	58	13.279	20.253	28.732	1.00 38.35	BLGL
MOTA	371	NZ	LYS	58	12.233	19.436	28.049	1.00 36.51 1.00 30.23	BLGL BLGL
MOTA	372	Ċ	LYS	58	17.726 17.564	19.135 19.064	29.969 28.753	1.00 30.23	BLGL
MOTA	373 374	Ŋ	CLU GLU	58 59	18.734	19.793	30.522	1.00 30.65	BLGL
MOTA MOTA	375	CA	GLU	59	19.722	20.483	29.709	1.00 31.60	BLGL
ATOM	376	CB	GLU	59	20.668	21.275	30.610	1.00 35.74	BLGL
ATOM	377	CG	GLU	59	19.971	22.381	31.397	1.00 42.93	BLGL
MOTA	378		GĽŰ	59	20.839	22.960		1.00 48.75	BLGL
MOTA	379		L GLU	59	20.327	23.818	33.264	1.00 51.01 1.00 51.49	BLGL BLGL
ATOM	380		2 GLU	59	22.026	22.558 19.493	32.638 28.862	1.00 30.47	BLGL
MOTA	381	C	GLU	59 59	20.511 21.086			1.00 30.17	BLGL
ATOM ATOM	382 383	O N	GLU ALA	60	20.531	18.235			BLGL
ATOM	384	CA	ALA	60	21.253			1.00 28.02	BLGL
ATOM	385	CB	ALA	60	21.611	16.065		1.00 29.83	BLGL
ATOM	386	C	ALA	60	20.461				BLGL
ATOM	387	0	ALA		20.975				BLGL BLGL
MOTA	388	N	GLY	61	19.208		27.269 26.167		BLGL
ATOM	389	CA	GLY		18.387 17.379		26.500		BLGL
ATOM	390	C	GLY		16.678				BLGL
MOTA MOTA	391 392		VAL		17.307				BLGL
ATOM	393				16.373			1.00 22.41	BLGL
ATOM	394	CB		62	16.738	13.577			BLGL
MOTA	395	CG	IAV I		15.754	12.514		1.00 22.01	BLGL
						_	4		

15.754 12.514 30.107 Fig. 4 cont.

132/174 18.146 13.018 29.664 1.00 20.65 BLGL CG2 VAL 62 ATOM 396 1.00 22.28 BLGL 14.658 28.230 62 14.958 С VAL MOTA 397 15.783 28.686 1.00 24.37 BLGL 398 0 VAL 62 14.743 MOTA BLGL 1.00 20.64 13.896 27.721 63 13.997 ASN ATOM 399 N BLGL 27,660 1.00 21.22 14.356 12.615 ATOM 400 CA ASN 63 26.204 1.00 20.41 BLGL 14.546 63 12.203 401 C8 ASN MOTA 25.349 1.00 20.90 BLGL 13.337 12.528 ATOM 402 CG ASN 63 1.00 22.33 25.723 BLGL 63 12.248 12.195 403 001 ASN MOTA BLGL .13.112 24.189 1.00 20.98 13.581 404 NO2 ASN 63 ATOM 1.00 21.56 BLGL 28.330 405 ASN 63 11.641 13.396 C ATOM BLGL 10.426 13.606 28.304 1.00 24.89 63 ASN ATOM 406 0 1.00 19.85 BLGL 12.346 28.939 MOTA 407 N TYR 64 12.171 1.00 18.37 BLGL 11.323 .11.360 29.578 64 408 TYR MOTA CA 1.00 18.15 BLGL 10.226 28.590 11.054 409 TYR Б4 ATOM CB 1.00 18.02 BLGL 64 9.601 10.025 28.244 ATOM 410 TYR CG BLGL 9.446 29.155 1.00 16.59 8.724 411 CD1 TYR 64 ATOM 1.00 17.75 BLGL 28.821 CZ1 TYR 64 7.397 9.210 ATOM 412 BLGL 9.109 10.375 26.985 1.00 20.14 64 ...ATOM 413 CD2 TYR BLGL 26.640 1.00 17.07 64 7.781 10.145 ATOM 414 CE2 TYR BLGL 64 ' 1.00 18.10 6.935 9.560 27.562 ATOM 415 CZ ' TYR 27.223 1.00 19.97 BLGL 9.301 Б4 5.634 ATOM 416 OH TYR BLGL 1.00 17.64 11.963 10.804 30.839 TYR 64 С MOTA 417 10.683 30.927 1.00 17.84 BLGL 13.181 418 0 TYR 64 ATOM BLGL 31.819 1.00 15.63 11.137 10.470 419 N VAL 65 ATOM 9.905 BLGL 65 11.644 33.050 1.00.16.50 VAL ATOM 420 CA 1.00 15.92 BLGL 10.909 34.215 VAL 65 11.567 ATOM 421 СВ 1.00 14.90 BLGL 11.909 10.207 35.522 65 422 CG1 VAL MOTA 12.536 33.975 1.00 14.25 BLGL 12.055 423 VAL 65 MOTA CG2 1.00 15.70 BLGL 10.847 8.668 33.414 MOTA 424 С VAL 65 1.00 16.30 BLGL 9.621 8.691 33.388 425 O VAL 65 ATOM 1.00 15.28 BLGL 33.740 11.548 7.587 ARG 66 MOTA 426 N 34.126 1.00 14.69 BLGL 10.898 6.343 ARG MOTA 427 CA 66 33.396 1.00 12.92 BLGL 11.520 5.145 ATOM 428 СВ ARG 66 1.00 16.36 BLGL 3.897 33.521 ARG 66 10.676 ATOM 429 CG BLGL 32.621 1.00 17.95 2.751 430 ARG 66 11.131 ATOM CD 1.00 21.82 BLGL 11.997 1.835 33.347 ARG MOTA 431 NE 66 1.00 20.23 BLGL 11.882 0.514 33.336 432 CZARG 66 ATOM 1.00.20.47 BLGL 32.628 10.933 -0.072 433 NH1 ARG 66 ATOM 12.720 -0.218 34.050 1.00 22.65 BLGL NH2 ARG 66 ATOM 434 35.627 1.00 15.52 BLGL 11.049 6:155 ATOM 435 С ARG 66 1.00 19.23 BLGL 12.097 6.461 36.194 436 ARG 66 MOTA 0 5.663 1.00 14.45 BLGL 10,003 36.277 437 VAL 67 ATOM N 1.00 14.29 BLGL 10.065 5.437 37.709 VAL 67 ATOM 438 CA 1.00 14.34 BLGL 6.591 38.500 ATOM 9.387 439 CB VAL 67 1.00 15.07 BLGL 8.010 6.866 37.946 440 CG1 VAL 67 ATOM 9.279 39.974 1.00 14.76 BLGL 6.226 CG2 VAL MOTA 441 67 38.050 1.00 13.80 BLGL 9.380 VAL 67 4.134 ATOM 442 ¢ BLGL 1.00 16.06 9,243 3.902 37.652 VAL 67 MOTA 443 0 10.084 BLGL 38.772 1.00 12.24 3.274 ATOM 444 ARG 68 N 1.00 13.36 BLGL 9.512 2.007 39.170 ARG 68 MOTA 445 CA 1.00 15.94 BLGL 10.613 0.987 39.505 MOTA 446 CB ARG 68 1.00 16.59 BLGL 40.530 11.653 1.445 447 ARG 68 MOTA CG 40.946 1.00 17.71 BLGL 12.582 0.299 ATOM 448 CD ARG 68 1.00 20.66 BLGL 0.787 41.717 ATOM 449 NE ARG 68 13.727 1.00 19.69 BLGL 1.365 41.187 14.806 MOTA 450 CZ ARG 68 1.00 18.60 1.00 19.53 BLGL · 15.791 1.788 41.964 NH1 ARG ATOM 451 68 BLGL 14.912 1.502 39.876 NH2 ARG ATOM 452 68 1.00 16.28 BLGL 40.383 2.250 MOTA 453 ARG 68 8.621 С 1.00 13.92 8.875 3.152 41.185 BLGL ARG 454 68 ATOM 0 1.449 1.00 16.59 BLGL 40.506 7.567 MOTA 455 14 ILE 69 1.00 17.08 BLGL 6.649 1.582 41.619 ILE 69 ATOM 456 CA 2.254 41.176 1.00 17.80 BLGL 5.331 ATOM 457 CB ILE 69 BLGL 1.00 16.20 4.442 2.505 42.392 ATOM 458 CG2 ILE 69 1.00 18.54 BLGL 5.634 3.577 40.463 ILE 69 ATOM 459 CG1 39.861. 1.00 16.60 BLGL 4.258 MOTA 460 CD1 ILE 69 4.420 BLGL 1.00 19.49

Fig. 4 cont.

0.224

6.326

69

ILE

ATOM

461

C

42.227

			•		13	3/174			
ATOM	462	0	ILE	69	5.851	-0.684	41.537	1.00 21.07	BLGL
MOTA	463	N	TRP	70	6.613	0.088	43.518	1.00 19.80	BLGL BLGL
ATOM	464	CA	TRP	70	6.329	-1.132	44.261	1.00 20.02	BLGL
MOTA	465	СВ	TRP	70 70	7.534 8.693	-1.548 -2.052	44.299	1.00 20.74	BLGL
MOTA	466	CD2	TRP TRP	· 70 70	10.078	-1.707	44.460	1.00 20.58	BLGL
MOTA MOTA	467 468	CE2		70	10.807	-2.445	43.496	1.00 20.35	BLGL
MOTA	469	CE3		70	. 10.774	-0.847	45.322	1.00 19.46	BLGL
MOTA	470		TRP	70	8.643	-2.958	43.278	1.00 20.51	BLGL
MOTA	471	NE1	TRP	70	9.906	-3.198	42.791	1.00 18.08	BLGL BLGL
MOTA	472	CZ2		70	12.200	-2.350	43.372	1.00 17.40 1.00 18.53	BLGL
ATOM	473		TRP	70 70	12.162 12.856	-0.752 -1.501	45.197 44.227	1.00 17.88	BLGL
MOTA	474 475	CH2 C	TRP TRP	70 -	5.145	-0.805	45.164	1.00 21.18	BLGL
ATOM ATOM	476	ò	TRP	70	5.010	0.328	45.626	1.00 20.39	BLGL
ATOM	477	N	ASN	71	4.279	-1.782	45.405	1.00 21.89	Brcr
MOTA	478	CA	ASN	71	3.105	-1.553	46.238	1.00 23.11	BLGL
A'TOM	479	СВ	ASN	71	2.204	-2.787	46.234	1.00 21.89	BLGL BLGL
MOTA	480	CG	ASN	71	. 1.600	-3.059 -8.325	44.875 43.907	1.00 24.42 1.00 24.93	BLGL
ATOM	481 .		ASN	71 71	2.312 0.277	-2.986	44.792	1.00 24.52	BLGL
MOTA MOTA	482 483	C	asn Asn	71	3.454	-1.182	47.673	1.00 23.89	BLGL
ATOM	484	õ	ASN	71	3.114	-0.093	48.150	1.00 23.65	BLGL
ATOM	485	N	ASP	72	4.139	-2.094	48.356	1.00 25.19	BLGL
MOTA	486	CA	ASP	72	4.531	-1.888	49.747	1.00 24.90	BLGL BLGL
ATOM	487	CB	ASP	72	3.576	-2.642	50.669	1.00 24.77 1.00 25.24	BLGL
ATOM	488	CG	ASP	72	3.706 3.494	-2.214 -3.063	52.105 52.990	1.00 25.24	BLGL
MOTA	489 490		ASP	. 72 72	4.006	-1.026	52.346	1.00 24.35	BLGL
ATOM ATOM	491	C	ASP	72	5.953	-2.384	49.997	1.00 24.58	BLGL
MOTA	492	ō	ASP	72	6.151	-3.472	50.538	1.00 25.47	BLGL
ATOM	493	N	PRO	. 73		-1.586	49.619	1.00 24.27	BLGL
MOTA	494	CD	PRO	73	6.856	-0.281	48.940	1.00 23.33 1.00 24.32	BLGL BLGL
ATOM	495	CA	PRO	73	8.366 9.091	-1.962 -1.009	49.805 48.866	1.00 24.32	BLGL
MOTA	496 497	CB	PRO PRO	73 73	8.272	0.237	49.001	1.00 23.40	BLGL
ATOM ATOM	497	C	PRO	73	8.863	-1.840	51.248	1.00 27.14	BLGL
ATOM	499	ŏ	PRO	73	9.987	-1.395	51.491	1.00 28.54	BLGL
ATOM	500	Ŋ	TYR	74	8.033	-2.233	52.208	1.00 27.12	BLGL
ATOM	501	CA	TYR		8.429	-2.147	53.609	1.00 26.57	BLGL BLGL
ATOM	502	СВ	TYR	74	7.838	-0.889 0.386	54.256 53.463	1.00 25.70 1.00 21.92	BLGL
ATOM ATOM	503	CG	TYR 1 TYR	74 74	8.022 7.148	0.721	52,427	1.00 22.26	BLGL
ATOM	504 505	CE.		74	7.304	1.909	51.707	1.00 21.83	BLGL
MOTA	506		2 TYR	74	9.057	1.265	53.758	1.00 18.92	BLGL
ATOM	507	CE	2 TYR	74	9.223	2,448	53.049	1.00 19.47	BLGL
MOTA	- 508	CZ	TYR	74	8.345	2.766	52.026	1.00 21.06	BLGL BLGL
MOTA	509	ОН		74	8.503	3.939	51.323 54.395	1.00 21.16 1.00 26.69	BLGL
MOTA	510 511	C	TYR TYR	74 74	7.970 7.119	-3.371 -4.131	53.928	1.00 26.70	BLGL
MOTA MOTA	512	<b>И</b> О	ASP	75	B.547	-3.568	55.579		BLGL
ATOM	513	CA	ASP	75	8.151	-4.687	56.422	1.00 25.66	BLGL
ATOM	514	СВ		75	9.348	-5.260	57.201		BLGL
MOTA	515	CG	ASP	75	9.948	-4.282			BLGL
ATOM	516		1 ASP	75	10.931	-4.668			BLGL BLGL
MOTA	517		2 ASP		9.455 7.060	-3.146 -4.208			BLGL
ATOM ATOM	518 519		ASP ASP		6.634	-3.063			BLGL
ATOM	520		ALA		6.602	-5.078		1.00 27.05	BLGL
ATOM	521				5.535	-4.722		1.00 28.91	BLGL
ATOM	522		ALA	76	5.304	-5.869			BLGL
MOTA	523		ALA		5.793	-3.438		1.00 29.89	BLGL BLGL
ATOM	524		ALA		4.873	-2.666			BLGL
MOTA	525		ASN		7.051 7.445	-3.213 -2.059			Brer
ATOM ATOM	526 527				8.619				BLGL
WT OLD	ا ے ب	ب	- 3 [1						

Fig. 4 cont.

### 134/174 -3.728 62.740 1.00 31.46 BLGL 8.337 528 ASN MOTA CG 62.659 1.00 35.40 BLGL 77 9.085 -4.700 OD1 ASN 529 MOTA BLGL -3.729 63.485 1.00 29.08 7.241 ATOM 530 ND2 ASN 77 60.294 1.00 30.14 BLGL 7.768 -0.802 77 ASN C MOTA 531 BLGL 8.048 0.249 60.874 1.00 31.47 77 ATOM 532 0 ASN BLGL 58.971 1.00 29.60 78 7.742 -0.906 GLY MOTA 533 N 7.998 58.146 1.00 30.47 BLGL 0.260 78 ATOM 534 CA GLY BLGL 1.00 30.69 57.665 GLY 78 9.422 0.434 ATOM 535 С BLGL 1.524 57.243 1.00 31.23 9.803 78 MOTA 536 0 GLY 57.735 1.00 30.64 BLGL -0.631 MOTA 537 ASN 79 10.212 N BLGL 79 11.599 -0.586 57.285 1.00 31.66 CA ASN ATOM 538 1.00 32.77 BLGL -1.618 58.043 12.437 MOTA 539 CB ASN 79 1.00 32.28 BLGL 59.539 79 12.478 -1.356 ASN 540 СG MOTA BLGL 1.00 31.97 -0.27759.981 79 12.875 541 OD1 ASN ATOM BLGL 1.00 29.86 60.325 ND2 ASN 79 12.074 -2:346 MOTA 542 BLGL 1.00 31.40 11.652 -0.888 55.788 79 MOTA 543 С ASN. 1.00 31.55 BLGL 55.352 -1.971 ATOM 544 O ASN 79 11.253 BLGL 1.00 30.48 12.146 0.072 55.013 80 GLY ATOM 545 N 53.573 1.00 28.01 BLGL -0.092 80 12.224 ATOM 546 CA GLY BLGL 1.00 26.92 80 13.066 -1.26553.132 GLY ATOM 547 С 53.737 1.00 28.09 BLGL 14.104 -1.544 80 ATOM 548 0 GLY BLGL 1.00 25.24 -1.958 52.089 81 12.611 TYR MOTA 549 N BLGL -3.110 51.539 1.00 24.70 550 TYR 81 13.330 MOTA CA 1.00 26.19 BLGL 50.559 .12.446 -3.891TYR 81 551 CB MOTA BLGL -4.704 11.309 51.155 1.00 28.51 MOTA CG TYR 81 552 50.324 1.00 30.98 BLGL -5.264 81 10.337 MOTA 553 CD1 TYR 1.00 33.39 BLGL -6.014 50.836 9.285 81 ATOM 554 CEL TYR 11.202 -4.919 52.525 1.00 27.25 BLGL 81 MOTA 555 CD2 TYR 1.00 30.71 BLGL 10.151 -5.673 53.053 ATOM CE₂ TYR 81 556 52.201 1.00 32.59 BLGL 9.191 -6.218 TYR 81 ATOM 557 CZ 52.701 1.00 29.32 BLGL 8.134 -6.95581 558 OH TYR MOTA BLGL 14.581 -2.643 50.791 1.00 23.17 ATOM 559 С TYR 81 50.411 1.00 22.30 BLGL -3,449 15.424 TYR 81 ATOM 560 0 BLGL 1.00 22.25 -1.337.50.575 82 14.692 MOTA 561 И GLY1.00 22.06 BLGL -0.812 49.863 15.840 82 562 CA GLY ATOM BLGL 1.00 23.07 15.544 -0.631 48.388 563 С GLY 82 MOTA BLGL 1.00 22.83 -0.466 47,994 0 GLY 82 14.392 MOTA 564 1.00 23.84 BLGL 47.561 16.582 -0.660 GLY 83 ATOM 565 N BLGL 46.133 16.384 -0.485 1.00 23.31 83 ATOM 566 CA GLY 1.00 23.19 BLGL 45.796 0.843 MOTA 567 С GLY 83 15.731 1.00 23.86 BLGL 44.693 1.024 15.219 568 GLY 83 MOTA 0 1.772 1.00 22.55 BLGL 15.740 46.748 569 N GLY 84 ATOM 1.00 18.60 BLGL 46.514 15.142 3.075 CA 84 ATOM 570 GLY BLGL 1.00 18.25 13.832 3.262 47.243 С GLY 84 ATOM 571 1.00 19.59 47.254 BLGL 13.282 4.354 84 572 0 GLY ATOM BLGL 47.867 1.00 18.82 13.339 2.199 85 MOTA 573 N ASN 1.00 22.71 BLGL 12.070 2.246 48.591 574 CA ASN 85 MOTA BLGL 1.00 22.20 3.011 49.914 12.217 ATOM 575 CB ASN 85 BLGL 50.902 1.00 24.42 2.319 85 13.143 ATOM 576 CG ASN 1.00 25.77 BLGL 13.320 1.102 50.869 85 MOTA 577 ODI ASN 13.721 1.00 25.80 BLGL 3.098 51.806 578 ASN 85 ATOM ND2 BLGL 47.729 1.00 23.49 11.004 2.929 85 579 ASN ATOM C 10.235 48.214 1.00 23.21 BLGL 3.761 580 O NZA 85 MOTA BLGL 1.00 23.70 46.452 ASN 86 10.950 2.566 581 N ATOM BLGL 10.001 45.546 1.00 24.44 3.196 ATOM 582 CA ASN 86 44.106 BLGL 10.447 1.00 21.35 86 3.008 583 CB ASN MOTA 1.00 21.48 BLGL 11.781 3.627 43.847 ASN 86 MOTA 584 CG BLGL 43.976 1.00 22.65 2.972 ASN 86 12,811 ATOM 585 OD1 1.00 20.47 BLGL 11.781 4.908 43.500 86 586 ND2 ASN MOTA 45.679 1.00 25.13 BLGL 2.785 ATOM 587 C ASN 86 8,546 BLGL 1.00 23.77 8.159 1.666 45.357 86 ASN 588 0 ATOM BLGL 7.742 46.155 1.00 25.52 3.723 ATOM 589 N ASP 87 1.00 26.02 BLGL 6,323 3.500 46.323 590 ASP 87 CA ATOM RLGL. 1.00 25.67 5.954 3.547 47.803 87 MOTA 591 CB ASP BLGL 1.00 30.07 48.524 592 CG ASP 87 6.584 4.724 ATOM

Fig. 4 cont.

5.705

6.994

87

ATOM

593

OD1 ASP

47.851

1.00 29.90

				•	. 13	5/174			
ATOM	594	OD2	ASP	87	6.656	4.668	49.771	1.00 31.21	BLGL
ATOM	595	C	ASP	87	5.625	4.613	45.566	1.00 25.13	BLGL
ATOM	596	0	ASP	87	6.276	5.396	44.877	1.00 25.07	BLGL
MOTA	597	N	LEU	88	4.307	4.693	45.694	1.00 25.05 1.00 27.31	BLGL BLGL
ATOM	598	CA	LEU	88		5.732 5.528	44.996 45.183	1.00 27.31	Brer
MOTA	599	CB	LEU	88 88	2.059 1.163	6.603	44.564	1.00 23.47	BLGL
ATOM	600 601	CG	LEU LEU	88	1.378	6.668	43.059	1.00 23.31	BLGL
ATOM ATOM	602		LEU	88	-0.283	6.294	44.880	1.00 23.48	BLGL
ATOM	603	C	LEU	88	3.956	7.146	45.440	1.00 28.05	BLGL
ATOM	604	0	LEU	88	3.942	8.072	44.633	1.00 28.88	BLGL
MOTA	605	N	GLU	89	4.310	7.312	46.713	1.00 28.47	BLGL
ATOM	606	CA	GLU	89	4.679	8.627	47.223	1.00 31.19 1.00 38.35	BLGL BLGL
MOTA	607	CB	GLU	89	4.884	8.596	48.743	1.00 38.33	BLGL
MOTA	608	CG	GLU	89	4.732 · 3.309	. 7.224 6.673	49.404 49.355	1.00 54.88	BLGL
MOTA	609 610	CD OF 1	GTN GTN	89 89	3.095	5.617	48.709	1.00 55.88	BLGL
ATOM ATOM	611		GLU	89	2.413	7,297	49.968	1.00 58.86	BLGL
MOTA	612	C	GLU	89	5.931	9.157	46.547	1.00 28.83	BLGL
ATOM	613	Ö.	GLU	89	5.958	10.293	46.083	1.00 29.30	BLGL
MOTA	614	N.	LYS	90	6.970	8.337	46.486	1.00 27.00	BLGL
MOTA	615	CA	LYS	90	8.202	8.758	45.833	1.00 25.31	BLGL BLGL
ATOM	616	СВ	LYS	90	9.308	7.731	46.074 47.526	1.00 24.21 1.00 23.42	BLGL
ATOM .	617 618	CG	LYS LYS	90 ·90	9.730 11.003	7.618 6.815	47.520	1.00 23.39	BLGL
ATOM ATOM	619	CE	LYS	90	11.521	6.845	49.092	1.00 22.77	BLGL
ATOM	620	NZ	LYS	90	10.589	6,181	50.039	1.00 24.27	BLGL
ATOM	621	C	LYS	90 ·	7.966	8.940	44.333	1.00 24.86	BLGL
ATOM	622	0	LYS	.90	8.604	9.779	43.696	1.00 23.88	BLGL
MOTA	623	N	ALA	91	7.043	8.157	43.776	1.00 22.89 1.00 23.29	BLGL BLGL
MOTA	624	CA	ALA	91	6.72 <b>7</b> 5.709	8.252 7.175	41,972	1.00 23.23	BLGL
ATOM ATOM	625 626	CB C	ALA ALA	91 91	6.172	9.644	42.060	1.00 23.82	BLGL
MOTA	627	Ö	ALA	91	6.501	10.244	41.042	1.00 24.10	$B\Gamma C\Gamma$
ATOM	628	N	ILE	92	5.335	10.154	42.956	1.00 24.44	BLGL
ATOM	629	CA	ILE	92	4.743	11.471	42.782	1.00 25.65	BLGL
MOTA	630	CB	ILE	92	3.549	11.651	43.748	1.00 26.69	BLGL BLGL
ATOM	631		? ILE	92	2.943 2.484	13.041 10.602	43.600 43.418	1.00 25.04 1.00 27.42	BLGL
ATOM ATOM	632 633		LILE	92 · 92	1.341	10.553	44.385	1.00 25.99	BLGL
ATOM	634	C.	ILE	. 92	5.794	12.568	42.992	1.00 25.95	BLGL
ATOM	635	0.	ILE	92	5.800	13.575	42.286	1.00 26.66	BLGL
ATOM	636	N	GLN	93	6.687	12.367	43.956	1.00 25.21	BLGL
MOTA	637	CA	GLN	93	7.746	13,332	44.206	1.00 25.19	BLGL
MOTA	638	CB	GLN	93	8.623	12.886	45.369 46.705	1.00 27.76 1.00 33.90	BLGL BLGL
ATOM	639	CD	GLN GLN	93 93	8.285 9.215	13.505 13.020	47.818	1.00 38.24	BLGL
ATOM ATOM	640 641		GLN	93	9,088	11.890	48.303	1.00 35.85	BLGL
ATOM	642		2 GLN	93	10.165	13.873	48.216	1.00 40-86	BLGL
MOTA	643	C	GLN	93	8.595	13.427	42.949	1.00 24.82	BLGL
ATOM	644	0	GLN	93	8.870	14.514	42.454	1.00 27.29	BLGL
MOTA	645	N	ILE	94	9.008	12.276	42.434	1.00 23.84	BLGL BLGL
MOTA	646	CA	ILE	94	9.818	12.225	41.223 40.929	1.00 21.73 1.00 20.65	BLGL
ATOM	647	CB	ILE 2 ILE	94 94	10.263 10.936	10.772 10.687	39.568	1.00 19.77	BLGL
mota Mota	648 649		1 ILE	94	11.202	10.293	42.043	1.00 18.55	BLGL
ATOM	650		1 ILE	94	11.644	8.866	41.914	1.00 12.93	BLGL
MOTA	651	C	ILE	94	9.027	12.770	40.038	1.00 21.61	BLGL
MOTA	652	0	ILE	94	9.545	13.553	39.232		BLGL
ATOM	653	N	GLY	95	7.764	12.362	39.955	1.00 22.02	BLGL BLGL
ATOM	654	CA	GLY	95 95	6.897 6.787	12.798 14.302	38.876 38.771		BLGL
atom Atom	655 656	CO	GLY GLY	95 95	6,787	14.302	37.683		BLGL
ATOM	657	N	LYS		6.526	14.947	39.907		BLGL
ATOM	658	CA			6.401	16.403	39.971	1.00 26.56	BLGL
ATOM	659	CB			6.095	16.844	41.401	1.00 26.83	BLGL

Fig. 4 cont.

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MOTA	660	CG	LYS	96	4.653	16.630	41.818	1.00 30.58	BLGL.
MOTA	661	CD	LYS	96	4.413	17.224	43.192 43.541	1.00 34.86 1.00 38.91	BLGL BLGL
ATOM	662	CE	LYS	96 96	2.939 2.712	17.256 17.810	44.909	1.00 38.31	BLGL
ATOM	663	NZ	LYS LYS	96. 96 ·	7.663	17.106	39.474	1.00 26.13	BLGL
ATOM	664 665	C 0	LYS	96 ·	7.592	18.041	38.676	1.00 25.77	BLGL
ATOM ATOM	666	N	ARG	97	8.818	16.649	39.946	1.00 26.45	BLGL
ATOM	667	CA	ARG	97	10.089	17.232	39.533	1.00 25.62	BLGL
MOTA	668	ÇВ	ARG	97	11.229	16.598	40.335	1.00 26.14	BLGL
MOTA	669	CĢ	ARG	97	11.105	16.909	41.824	1.00 28.26	BLGL
MOTA	670	CD	ARG	97	12.157	16.228	42.687 42.385	1.00 28.70 1.00 30.96	BLGL BLGL
MOTA	671	NE	ARG	97	13.514	16.674 16.211	42.363	1.00 29.36	BLGL
ATOM	672	CZ	ARG ARG	97 97	14.593	15.297	43.959	1.00 26.96	BLGL
MOTA MOTA	673 674		ARG	97	15.799	16.650	42.671	1,00 26.20	BLGL
ATOM	675	C	ARG	97 ·	10.310	17.060	38.032	1.00 24.94	BLGL
ATOM	676	ō	ARG	97	10,778	17.973	37.354	1.00 24.07	BLGL
ATOM	677	N	ALA ·	98	9.959	15.890	37.510	1.00 24.88	BLGL
MOTA	678	CA	ALA	98	10.104	15.626	36.084	1.00 24.73	BLGL
ATOM	679	CB	ALA	98 •	9.673	14.198	35.771	1.00 26.89	BLGL BLGL
ATOM	680	С	ALA	. 98	9.265	16.620	35.277 34.256	1.00 24.32 1.00 21.35	BLGL
MOTA	681	0	ALA	98 99	9.715 B.041	17.145 16.875	35.727	1.00 25.11	BLGL
ATOM .	682 683	N CA	ASN ASN	99	7.196	17.830	35.019	1.00 27.26	BLGL
ATOM .	684	СВ	ASN	99	5.802	17.871	35.601	1.00 29.92	BLGL
ATOM	685	CG	ASN	99	5.039	16.631	35.330	1.00 36.77	BLGL
MOTA	686	ODl	NZA	99	3.817	16.649	35.364	1.00 43.97	BLGL
MOTA	687	ND2	ASN	99	5.743	15.529	35.063	1.00 38.67	BLGL
ATOM	688	С	ASN	99	7.766	19.229	35.096	1.00 26.84	BLGL BLGL
MOTA	689	0	ASN	99	7.850 8.143	19.919 19.652	34.090 36.298	1.00 23.90	BLGL
MOTA	690 691	N	ALA ALA	100 100	8.689	20.982	36.481	1.00 23.21	BLGL
atom atom	692	CA CB	ALA	100	9.214	21.137	37.894	1.00 20.39	BLGL
ATOM	693	C	ALA	100	9.800	21.244	35.470	1.00 25.29	BLGL
MOTA	694	ō	ALA	100	10.088	22.394	35.141	1.00 26.23	BLGL
ATOM	695	N	ASN	101	10.409	20.174	34.963	1.00 25.14	BLGL
MOTA	696	CA	ASN	101	11.492	20.307	33.998	1.00 25.17	BLGL
MOTA	697	CB	ASN	101	12,696	19.515	34.483	1.00 24.95 1.00 25.85	BLGL BLGL
MOTA	698	CG	ASN	101	13.280	20.091 21.145	35.747 35.719	1.00 29.40	BLGL
MOTA	699 700	ND2		101 101	13.914 13.054	19.422	36.868	1.00 24.97	
MOTA MOTA	701	C	ASN	101	11.118	19.898	32.582	1.00 25.90	BLGL
ATOM	702	ō	ASN	101	11.978	19.563	31.772	1.00 27.14	BLGL
ATOM	703	N	GLY	102	9.824	1,9.932	32.290	1.00 25.80	BLGL
ATOM	704	CA	GLY	102	9.345	19.598	30.962	1.00 24.78	BLGL
MOTA	705	С	GLY	102	9.671	18.215	30.447	1.00 25.83	BLGL BLGL
ATOM	706	0	GLY	102	10.048	18.061	29.289 31.297	1.00 27.54	BLGL
MOTA	707	N	MET	103 103	9.525 9.793	17.205 15.827	30.899	1.00 26.04	BLGL
ATOM	708 709	CA CB	MET MET		11.006	15.283	31.662	1.00 26.48	BLGL
atom Atom	710	CG	MET	103	12.265	16.110	31.451	1.00 29.27	BLGL
ATOM	711	SD	MET		13.767	15.380	32.124	1.00 31.74	BLGL
MOTA	712	CE	MET		13.716	16.017	33.804	1.00 31.73	BLGL
MOTA	713	С	MET	103	8.559	14.978	31.191	1.00 25.31	BLGL
MOTA	714	0	MET		7.892		32.206		BLGL BLGL
MOTA	715	N	LYS		8.243		30.294		BLGL
MOTA	716	CA	LYS LYS		7.082 6.668		30.484 29.167		BLGL
ATOM	717 718	CB CG	LYS		6.265				BLGL
ATOM ATOM	718	ÇD	LYS		4.800				BLGL
MOTA	720		LYS		4.294				BLGL
ATOM	721	NZ	LYS		2.807		26.870	1.00 40.79	BLGL
ATOM	722		LYS		7.452	12.075			BLGL
ATOM	723	0	LYS		8.632			1.00 23.51	BLGL
MOTA	724		LEU		6.450				BLGL BLGL
MOTA	725	CA	LEU	105	6.705	10.313	32.955	1.00 19.77	2101
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Fig. 4 cont.

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ATOM	726	CB	LEU	105	5.975	10.559	34.279	1.00 18.76	BLGL
ATOM	727	CG	LEU	105	6.334	9.548	35.381	1.00 19.18	BLGL
ATOM	728	CD1	LEU	105	7.586	10.007	36.100	1.00 16.56	BLGL
ATOM	729	CD2		105	5.195	9.412	36.364	1.00 21.13	BLGL
ATOM	. 730	C	LEU	105	6.280	8.941	32.418	1.00 19.86	BLGL
	731	ŏ	LEU	105	5.285	8.812	31.701	1.00 16.96	BLGL
ATOM			LEU.	106	7.059	7.920	32.758	1.00 19.88	BLGL
ATOM	732	N		106	6.738	6.551	32.381	1.00 19.92	BLGL
MOTA	.733	CA	LEU			5.878	31.637	1.00 17.61	BLGL
MOTA	734	CB	LEU	106	7.889			1.00 21.29	BLGL
Mota	735	CG	<b>LEU</b>	106	7.550	4.607	30.838	1.00 21.25	BLGL
ATOM	736	CD1	LEU	106	8.845	3.872	30.511		BLGL
ATOM	737	CD2	<b>LEU</b>	106	6.627	3.689	31 604	1.00 17.96	
ATOM	738	С	LEU	106	6.567	5.877	33.730	1.00 19.81	BLGL
ATOM	739	0	LEU	106	7.546 ·		34.437	1.00 19.58	BLGL
ATOM	740	N	ALA	107	5.327	5.581	34.102	1.00 20.44	BLGL
MOTA	741	CA	ALA	107	5.052	4.922	35.373	1.00 20.99	BLGL
ATOM	742	СВ	ALA	107	3.634	5.240	35.826	1.00 21.52	BLGL
ATOM	743	C	ALA	107	5.224	3.418	35.177	1.00 21.97	BLGL.
ATOM	744	Õ	ALA	107	4.493	2,796	34:406	1.00 23.04	BLGL .
	745	N	ASP	108	6.192	2.828	35.867	1.00 21.22	BLGL
ATOM	746		ASP	108	6.438	1.400	35.726	1.00 20.00	BLGL
MOTA			ASP	108	7.932	1.175	35.463	1.00 17.66	BLGL
ATOM	747	CB				-0.289	35.455	1.00 17.79	BLGL
MOTA	748	CG	ASP	108	8.327	-1.173	35.519	1.00 16.92	BLGL
MOTA	749		ASP	108	7.448	-		1.00 18.27	BLGL
MOTA	750		ASP.	108	9.542	-0.562	35.385	1.00 21.24	Brcr
ATOM	751	С	ASP	108	5.966	0.625			BLGL
MOTA	752	0	ASP	108	6.635	0.614	37.984	1.00 25.51	
ATOM	753	N	PHE	109	4.801	-0.010	36.840	1.00 19.98	BLGL
MOTA	754	CA	PHE	109	4.256	-0.792	37.939	1.00 20.05	BLGL
ATOM	755	CB	PHE	109	2.739	-0.903	37.850	1.00 20.06	BLGL
ATOM	756	CG	PHE	109	2.033	0.386	38.066		BLGL
ATOM	757		PHE	109	1.751	1.225	36.995	1.00 21.28	BLGL
ATOM	758		PHE	109	1.665	0.777	39.349	1.00 21.79	BLGL
ATOM	759		PHE	109	1.110	2.442	37.194	1.00 24.40	BLGL
ATOM	760		PHE	109	1.026	1.989	39.564	1.00 23.03	BLGL
ATOM	761	CZ	PHE	109	0.745	2.828	38.482	1.00 23.74	BLGL
	762	C	PHE	109	4.822	-2.190	37.949	1.00 19.77	BLGL
MOTA		٥	PHE	109	4.680	-2,932	36.978	1.00 18.81	BLGL
ATOM	763			110	5.464	-2.547	39.054	1.00 19.76	BLGL
MOTA	764	Ŋ	HIS		6,023	-3.875	39.188	1.00 20.72	BLGL
MOTA	765	CA	HIS	110		-3.876	40.157	1.00 20.31	BLGL
ATOM	766	CB	HIS	110.	7.207		39.540	1.00 20.23	BLGL
MOTA	767	CG	HIS	110	8.497	-3.439		1.00 19.83	BLGL
ATOM	768		HIS	110	8.779	-2.456			BLGL
MOTA	769		. HIS	110	9.703	-4.034	39.845	1.00 21.63	
ATOM	770		HIS	110	10.671	-3.437	_	1.00 20.13	BLGL
MOTA	771	NE2	HIS	110	10.137	-2.475		1.00 20.13	BLGL
ATOM	772	С	HIS	110	4.948	~4.823		1.00 20.55	BLGL
ATOM	773	0	HIS	110	5.056	-6.036		1.00 20.58	BLGL
ATOM	774	N	TYR	111	3.900	-4.267		1.00 21.08	BLGL
ATOM	775	ÇA	TYR	. 111	2.827	-5.093	40.830	1.00 23.38	BLGL
ATOM	776	CB	TYR	111	2.039	-5.759	39.695		BLGL
ATOM	777	CG	TYR	111	1.274	-4.758	38.858	1.00 23.84	BLGL
ATOM	778		TYR	111	1.551	-4.593	37.501	1.00 22.76	BLGL
	779		LTYR	111	0.878	-3.641			BLGL
MOTA	780		TYR	111	0.297	-3.945			BLGL
MOTA					-0.378	-2.991			BLGL
ATOM	781		2 TYR			-2.844			BLGL
ATOM	782	CZ	TYR		-0.082				BLGL
ATOM	783	OH	TYR		-0.738	-1.887			BLGL
ATOM	784	C	TYR	111	3.439	-6.137			
ATOM	785	0	TYR		3.094	-7.317			BLGL
MOTA	786	11	SER	112	4.372	-5.668			BLGL
MOTA	787	CA	SER	112	5.071	-6.493			BLGL
MOTA	788	CB	SER	112	6.249	-7.201			Brcr
ATOM	789		SER		7.002	-7.894	43.866	1.00 23.73	BLGL
ATOM	790		SER		5.585	-5.542	44.601		Brcr
ATOM	791		SER		5.631				BLGL
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Fig. 4 cont.

					1	38/174			
ATOM	792	N	ASP	113	5.968	-6.069	45.760	1.00 22.31	BLGL
ATOM	793		ASP	113	6.486	-5.208	46.815	1.00 22.28 1.00 22.82	BLGL BLGL
ATOM	794		ASP	113	6.202	-5.795 -5.719	48.199 48.577	1.00 25.54	BLGL
MOTA	795	-	ASP	113 113	4.732 4.032	-4.825	48.056	1.00 23.47	BLGL
ATOM	796 797	·ODZ	ASP	113	4.281	-6.544	49.406	1.00 24.91	BLGL
MOTA: MOTA:	798	C	ASP	113	7.982	-4.969	46.651	1.00 21.86	BLGL
ATOM	799	o	ASP	113	8.548	-4.101	47.309	1.00 21.62	BLGL
ATOM	800	N	PHE	114	8.622		45.775	1.00 20.23	BLGL
MOTA	801	CA	PHE	114	10.046		45.547	1.00 20.78	BLGL BLGL
MOTA	802	CB	PHE	114	10.853		46.549 46.838	1.00 21.28 1.00 24.03	BLGL
ATOM	803	CG	PHE	114	12.221 12.420		46.919	1.00 24.35	BLGL
MOTA	804 805	CD1		114 114	13.308		47.064	1.00 24.49	BLGL
MOTA MOTA	B06	CE1		114	13.684	_	47.224	1.00 22.80	BLGL
ATOM	807	CE2		114	14.575		47.372	1.00 20.26	BLGL
MOTA	808	CZ	PHE	114	14.761		47.451	1.00 20.45	BLGL
ATOM	809	С	PHE	114	10.392		44.122	1.00 21.41	BLGL BLGL
MOTA	810		PHE	114	9.507		43.361 43.768	1.00 21.59 1.00 20.29	BLGL
MOTA	811	И	TRP	115.	11:675 12.152		42.418	1.00 19.28	BLGL
MOTA	812 813	CA CB	TRP TRP	115 115	13.634		42.445	1.00 20.57	BLGL
MOTA MOTA	814	CG	TRP	115	14.575		42.963	1.00 21.03	BLGL
ATOM	815		TRP	115	14.942		42.311.	1.00 20.71	BLGL
ATOM	816		TRP	115	15.786		43.198	1.00 21.97	BLGL
MOTA	817		TRP	115	14.637		41.066	1.00 20.82	BLGL BLGL
MOTA	818		TRP	115	15.202		44.177 44.328	1.00 19.55 1.00 18.99	BLGL
MOTA	819		TRP	115 115	15.929 16.329		44.328	1.00 22.16	BLGL
MOTA MOTA	820 821		TRP TRP	115	15.177		40.746	1.00 21.59	BLGL
MOTA	822		TRP	115	16.013		41.653	1.00 22.47	. BLGL
ATOM	823	С	TRP	115	11.36	-7.231	41.665	1.00 18.82	BLGL
MOTA	824	0	TRP	115	11.090		42.193	1.00 17.18	BLGL
MOTA	825	N	ALA	116	10.999		40.426	1.00 17.42	BLGL BLGL
MOTA	826	CA	ALA	116	10.27	_	39.589 39.223	1.00 19.55 1.00 18.74	BLGL
ATOM	827	CB C	ALA ALA	116 116	8.914 11.110		38.331	1.00 22.25	BLGL
ATOM ATOM	828 829	. 0	ALA	116	11.45		37.631	1.00 25.39	BLGL
ATOM	830	N	ASP	117	11.45	_	38.051	1.00 21.71	BLGL
ATOM	831	CA	ASP	117	12.24		36.872	1.00 22.29	BLGL
ATOM	832	CB	ASP	117	13.73		37.209	1.00 22.60	BLGL BLGL
ATOM	833	CG	ASP	117		4 -10.578		1.00 26.69 1.00 29.56	BLGL
ATOM	834	-	ASP	117 117		2 -11.738 7 -10.171	39.190	1.00 30.52	BLGL
atom atom	835 836	C	ASP	117		3 -11.045		1.00 22.91	BLGL
ATOM	837	ŏ	ASP	117		0 -11.601		1.00 24.06	BLGL
MOTA	838	И	PRO	118	12.61	7 -11.619	35.409	1.00 22.06	BLGL
ATOM	839	CD	PRO	118	13.73	4 -11.056	34.639	1.00 20.93	BLGL
ATOM	840	CA	PRO	118	12.25	2 -12.935	34.880	1.00 24.27 1.00 22.87	BLGL BLGL
MOTA	841	CB	PRO	118		1 -13.176 9 -11.821			BLGL
ATOM	842	CG	PRO	118 118		2 -14.077		1.00 26.00	BLGL
MOTA MOTA	843 844	C O	PRO	118		7 -15.140			BLGL
MOTA	845	N	ALA	119		5 -13.868		1.00 28.00	BLGL
ATOM	846	CA	ALA	119		2 -14.917		1.00 28.48	BLGL
ATOM	847	CB	ALA	119		6 -15.188			BLGL
ATOM	848	C	ALA	119		9 -14.568			BLGL BLGL
ATOM	849	0	ALA	119		7 -15.447			BLGL
ATOM	850	N	LYS	120 120		,9 -13.279 :0 -12.842			BLGL
ATOM ATOM	851 852	CA CB	LYS LYS	120		$\frac{10}{3}$ $-12.032$			BLGL
ATOM	853		LYS			0 -12.838		1.00 38.25	BLGL
ATOM	854		LYS	120		7 -12.000		1.00 40.66	BLGL
ATOM	855		LYS	120	14.80	1 -11.115	42.222	1.00 44.93	BLGL
MOTA	856	NZ	LYS			7 -10.373			BLGL BLGL
ATOM	857	С	LYS	120	9.70	08 -12.020	40.224	1.00 28.61	וופונט
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Fig. 4 cont.

ATOM	858	0	LYS	120	9.841 -	10.912	39.702	1.00 28.45	BLGL
ATOM	859	N	GLN	121	8.525 -	12.589	40.425	1.00 26.27	BLGL
MOTA	860	CA	GLN	121	7.273 -	11.913	40.108	1.00 25.49	BLGL
ATOM	861	СВ	GLN	121	6.673 -	-12.457	38.805	1.00 24.33	BLGL
ATOM	862	CG	GLN	121	7.392 -		37.525	1.00 20.53	BLGL
ATOM	863	CD	GLN	121	7.376 -		37.291	1.00 18.36	BLGL
MOTA	864	OE1	GLN	121	6.425	-9.838	37.659	1.00 15.80	BLGL
MOTA	865	NE2	GLN	121	8.424 -		36.655	1.00 17.37	BLGL BLGL
ATCM	866	С	GLN	121		-12.176	41.281	1.00 25.36	BLGL
MOTA	867	0	GLN	121		-12.571	41.099	1.00 26.22 1.00 25.47	BLGL
MOTA	868	N	LYS	122		-11.970	42.489 43.716	1.00 25.47	BLGL
MOTA	869	CA	LYS	122		-12.188	43.716	1.00 27.22	BLGL
MOTA	870	СВ	LYS	122		-12.079 -12.412	44.324	1.00 29.39	BLGL
MOTA	871	CG	LYS	122		-13.759	46.785	1.00 32.32	BLGL
ATOM	872	CD	LYS	122		-13.609	47.961	1.00 31.56	BLGL
ATOM	873	CE	LYS	122 122		-12.997	49.160	1.00 32.62	BLGL
ATOM	874	ΝZ	LYS	122		-11.162	43.833	1.00 26.53	BLGL
MOTA	875 876	C	LYS	122	5.151	-9.988	43.504	1.00 28.15	BLGL
ATOM	-876	0	LYS	123		-11.603	44,298	1.00 25.34	BLGL
ATOM	877 879	N CA	ALA ALA	123		-10.700	44.449	1.00 24.78	BLGL
MOTA	878 879	CB	ALA	123		-11.491	44.559	1.00 24.09	BLGL
atom Atom	880	С	ALA	123	2.830	-9.820	45.675	1.00 23.46	BLGL
ATOM	881	ŏ	ALA	123		-10.177	46.622	1.00 23.28	BLGL
MOTA	882	N	PRO	124	2.212	-8.636	45.660	1.00 23.79	BLGL
ATOM	883	CD	PRO	124	1.484	-7.998	44.548	1.00 21.21	BLGL
MOTA	884	CA	PRO	124	2.310	-7.738	46.811	1.00 22.77	BLGL
ATOM .	. 885	CB	PRO	124	1.392	-6.588	46.419	1.00 21.28	BLGL
ATOM	886	CG	PRO	124	1.521	-6.547	44.927	1.00 19.51	BLGL
ATOM	887	С	PRO	124	1.791	-8.491	48.037	1.00 23.09	BLGL
MOTA	888	0	PRO	124	0.883	-9.312	47.922	1.00 22.17	BLGL BLGL
ATOM	889	N	LYS	125	2.360	-8.228	49.205	1.00 25.24	BLGL
ATOM	890	CA	LYS	125	1.910	-8.916	50.411	1.00 25.84	BLGL
MOTA	891	CB	LYS	125	2.612	-8.350	51.656	1.00 23.65	BLGL
ATOM	892	CG	LYS	125	4.109	-8.642	51.733 52.990	1.00 21.46 1.00 15.25	BLGL
MOTA	893	CD	LYS	125	4.750	-8.067	53.029	1.00 13.23	BLGL
ATOM	. 894	CE	LYS	125	4.683 5.440	-6.554 -5.911	51.912	1.00 20.44	BLGL
ATOM	895	NZ	LYS	125 125	0.391	-8.807	50.570	1.00 27.21	BLGL
ATOM	896	C	LYS LYS	125	-0.264	-9.763	50.976	1.00 27.46	BLGL
ATOM	897 8 <b>98</b>	O N	ALA	126		-7.651	50.232	1.00 27.45	BLGL
ATOM ATOM	899	CA	ALA	126	-1.608	-7.438	50.360	1.00 28.44	BLGL
MOTA	900	CB	ALA	126	-1.942	-5.996	_	1.00 27.50	BLGL
MOTA	901	c	ALA	126	-2.445	-8.367	49.487	1.00 30.46	BLGL
MOTA	902	ŏ	ALA	126	-3.578	-8.700	49.835	1.00 32.72	$\mathtt{BLGL}$
ATOM	903	N	TRP	127	-1.893	-8.780	48.352	1.00 31.67	BLGL
ATOM	904	CA	TRP	127	-2.608	-9.663	47.436	1.00 32.34	BLGL
MOTA	905	CB	TRP	127	-2.274	-9.301		1.00 29.98	BLGL
ATOM	906	CG	TRP	127	-2.525			1.00 26.78	BLGL
MOTA	907	CD	2 TRP	127	-2.176	-7.215		1.00 25.87	BLGL
ATOM	908		2 TRP	127	-2.582	-5.869	_		BLGL
MOTA	909	CE	3 TRP	127	-1.558	-7.643		1.00 25.70	BLGL
MOTA	910		1 TRP	127	-3.116				BLGL BLGL
MOTA	911		1 TRP	127	-3.153				Brer
ATOM	912		2 TRP	127	-2.390				BLGL
ATOM	913		3 TRP	127	-1.367				. BLGL
MOTA	914		2 TRP	127	-1.781				BLGL
ATOM	915		TRP	127		-11.113			BLGL
ATOM	916		TRP	127		-12.039 -11.284			BLGI
ATOM	917		ALA	128		-12.589			BLGI
MOTA	918			128 128		-12.528		<b>-</b> -	BLGI
ATOM	919		ALA ALA	128		-13.759			BLGI
ATOM ATOM	920 921		ALA	128		-14.671			BLGI
ATOM	922		ASN	129		-13.751		1.00 40.50	BLGI
ATOM	923			129		-14.836			BLGI
117 011	243								

Fig. 4 cont.

					140/117	
ATOM	924	CB	asn	129	-3.794 -15.632 50.788 1.00 47.42	BLGL
ATOM	925	_	ASN	129	-3.746 -14.751 52.018 1.00 50.55 -3.975 -13.545 51.941 1.00 54.24	BLGL BLGL
ATOM	926	ODl		129	-3.975 -13.545 51.941 1.00 54.24 -3.460 -15.356 53.168 1.00 50.85	BLGL
ATOM	927	ND2	ASN	129 129	-5.107 -14.380 49.047 1.00 44.76	BLGL
atom Atom	928 929		ASN	129	-6.070 -14.460 49.813 1.00 45.16	BLGL
MOTA	930	N	LEU	130	-5.194 -13.901 47.810 1.00 44.30	BLGL
ATOM	931	CA	LEU	130	-6.452 -13.456 47.230 1.00 43.76	BLGL
MOTA	932	CB	LEU	130	-6.341 -12.018 46.731 1.00 44.19	BLGL
MOTA	933	CG	LEU	130	-6.396 -10.901 47.767 1.00 44.74 -6.258 -9.564 47.071 1.00 45.24	BLGL BLGL
ATOM	934	CD1		130	-6.258 -9.564 47.071 1.00 45.24 -7.712 -10.970 48.515 1.00 45.37	BLGL
ATOM	935 936	CD2 C	LEU	130 130	-6.727 -14.363 46.049 1.00 43.61	BLGL
ATOM ATOM	937	o	LEU	130	-5.801 -14.769 45.351 1.00 43.36	BLGL
ATOM	938	N	ASN	131	-7.991 -14.695 45.823 1.00 44.12	BLGL -
MOTA	939	CA	ASN	131	-8.318 -15.549 44.690 1.00 44.97	BLGL
MOTA	940	CB	NEA	131	-9.757 -16.078 44.801 1.00 47.76	BLGL BLGL
ATOM	941	CG	ASN	131	-10.794 -14.976 44.772 1.00 51.05 -10.669 -13.968 45.465 1.00 55.52	BLGL
MOTA	942	OD1	ASN ASN	131 131	-10.669 -13.968 45.465 1.00 55.52 -11.835 -15.170 43.977 1.00 52.37	BLGL
ATOM ATOM	943 944	C	ASN	131	-8.133 -14.706 43.436 1.00 43.17	BLGL
ATOM	945	Õ	ASN	131	-8.381 -13.502 43.451 1.00 42.05	BLGL
ATOM	946	N	PHE	132	-7.682 -15.338 42.360 1.00 42.47	BLGL
MOTA	947	CA	BHE	132	-7.440 -14.638 41.107 1.00 42.04	BLGL
ATOM	948	CB	PHE	132		BLGL BLGL
MOTA	949	CG	PHE	132	-7.126 -14.971 38.633 1.00 42.75 -5.870 -14.426 38.396 1.00 42.49	BLGL
ATOM ATOM	950 951		PHE	132 132	-8.103 -14.855 37.656 1.00 43.76	BLGL
ATOM	952		PHE	132	-5.594 -13.769 37.204 1.00 42.79	BLGL
ATOM	953		PHE	132	-7.834 -14.197 36.455 1.00 44.60	BLGL
ATOM	954	CZ	PHE	132	-6.579 -13.655 36.232 1.00 43.31	BLGL
ATOM	955	С	PHE	132	-8.439 -13.523 40.808 1.00 41.68 -8.050 -12.415 40.445 1.00 41.50	, BLGL BLGL
ATOM	956	0	PHE	132	-8.050 -12.415 40.445 1.00 41.50 -9.725 -13.815 40.951 1.00 42.52	BLGL
MOTA	957 958	n Ca	GTO GTO	133 133	-10.759 -12.821 40.691 1.00 42.35	BLGL
ATOM ATOM	959	CB	GLU	133	-12.138 -13.409 40.985 1.00 46.23	BLGL
ATOM	960	CG	GLU	133	-12.591 -14.433 39.967 1.00 53.21	BLGL
ATOM	961	CD	GLU	133	-12.550 -13.879 38.553 1.00 57.33	BLGL
MOTA	962		GLU	133	-13.059 -12.757 38.347 1.00 58.31 -12.015 -14.564 37.652 1.00 61.34	BLGL BLGL
ATOM	963		GLU	133	-12.015 -14.564 37.652 1.00 61.34 -10.573 -11.542 41.500 1.00 40.12	BLGL
MOTA MOTA	964 965	0	GLU	133 133	-10.654 -10.443 40.951 1.00 38.25	BLGL
ATOM	966	Ŋ	ASP	134	-10.326 -11.691 42.800 1.00 38.18	BLGL
ATOM	967	CA	ASP	134	-10.133 -10.547 43.684 1.00 37.03	BLGL
ATOM	968	CB	ASP	134	-10.203 -10.994 45.142 1.00 39.68	BLGL
MOTA	969	CG	ASP	134	-11.625 -11.128 45.640 1.00 40.58 -11.816 -11.683 46.744 1.00 40.76	BLGL BLGL
ATOM	970		ASP	134 134	-11.816 -11.683 46.744 1.00 40.76 -12.546 -10.666 44.930 1.00 42.41	BLGL
MOTA MOTA	971 972	C	ASP ASP	134	-8.816 -9.822 43.434 1.00 34.44	BLGL
ATOM	973	õ	ASP	134	-8.710 -8.611 43.633 1.00 33.65	BLGL
MOTA	974	N	LYS	135	-7.810 -10.570 43.003 1.00 32.43	BLGL
MOTA	975	CA	LYS	135	-6.510 -9.989 42.717 1.00 30.17	BLGL
MOTA	976		LYS	135	-5.468 -11.092 42.537 1.00 28.01 -4.058 -10.568 42.377 1.00 25.79	BLGL BLGL
ATOM	977	CG	LYS	135	-4.058 -10.568 42.377 1.00 25.79 -3.090 -11.647 41.928 1.00 24.80	BLGL
ATOM	978 979		LYS LYS	135 135	-2.994 -12.773 42.922 1.00 24.10	BLGL
ATOM ATOM	980		LYS		-1.961 -13.742 42.491 1.00 24.21	BLGL
MOTA	981		LYS	135	-6.615 -9.147 41.443 1.00 29.06	BLGL
ATOM	982	0	LYS	135	-6.092 -8.032 41.384 1.00 29.12	BLGL
ATOM	983		LYS		-7.303 -9.682 40.436 1.00 28.19	BLGL
MOTA	984		LYS		-7.492 -8.986 39.166 1.00 26.63 -8.364 -9.819 38.220 1.00 28.55	BLGL BLGL
MOTA	985		LYS		-8.364 -9.819 38.220 1.00 28.55 -8.455 -9.248 36.811 1.00 33.70	BLGL
ATOM ATOM	986 987		LYS LYS		-9.739 -9.661 36.093 1.00 40.26	BLGL
MOTA	988		LYS		-9.825 -11.171 35.873 1.00 44.05	BLGL
ATOM	989		LYS		-11.113 -11.590 35.228 1.00 44.46	BLGL

Fig. 4 cont.

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ATOM	990	С	LYS	136	-8.149	-7.627	39.408	1.00 24.62	BLGL
MOTA	991	ō	LYS	136		-6.611	38.868	1.00 24.91	BLGL
	992	N	THR	137	-9.197	-7.607	40.221	1.00 23.73	BLGL
ATOM	993	CA	THR	137	-9.874	-6.356	40.519	1.00 24.53	BLGL
MOTA	994	CB	THR	137	-11.262	-6.603	41.168	1.00 26.21	BLGL
MOTA	995		THR	137	-11.679	-5.422	41.855	1.00 28.27	BLGL
MOTA	996		THR	137	-11.220	-7.759	42.134	1.00 27.71	BLGL
ATOM	9.97	C	THR	137	-9.017	~5,451	41,412	1,00 24.00	BLGL
MOTA	998	0	THR	137	-9.108	-4.221	41.334	1.00 23.13	BLGL
ATOM	999	И	ALA	138	-8.174	-6.054	42.248	1.00 22.08	BLGL
MOTA	1000	CA	ALA	138	-7.289	-5.277	43.115	1.00 23.30	BLGL
ATOM ATOM	1000	CB	ALA	138	~6.612	-6.182	44.128	1.00 19.73	BLGL
ATOM MOTA	1002	C		. 138	-6.228	-4.570	42,265	1.00 23.73	BLGL
MOTA	1003	ō	ALA	138	-5.896	-3.401	42.497	1.00 23.84	BLGL
ATOM	1004	N	LEU	139	-5.700	-5.288	41.280	1.00 21.33	BLGL
MOTA	1005	CA	LEU	139	-4.690	-4.729	40.402	1.00 22.61	BLGL
ATOM	1006	СВ	LEU	139	-4.144	-5.806	39.460	1.00 21.44	$\mathtt{BLGL}$
ATOM	1007	CG	LEU	139	~2.895	-5.411	38.656	1.00 21.68	BLGL
MOTA	1008		LEU	139	-2.111	-6.664	38.340	1.00 22.58	BLGL
ATOM	1009		LEU	139	-3.265	-4.658	37.383	1.00 17.55	BLGL
ATOM	1010	C	LEU	139	-5.280	-3.576	39.603	1.00 23.36	BLGL
MOTA	1011	ŏ	LEU	139	-4.629	-2.550	39.401	1.00 23.02	BLGL
ATOM	1012	N	TYR	140	-6.513	-3.747	39.141	1.00 24.62	BLGL
ATOM	1013	CA	TYR	140	-7.176	-2.697	38.381	1.00 25.60	BLGL
MOTA	1014	CB	TYR	140	-8.514	-3.206	37.833	1.00 23.98	BLGL
ATOM	1015	CG	TYR	140	-9.494	-2.109	37.498	1.00 22.17	BLGL
ATOM	1016		TYR	140	-10.389	-1.634	38.452	1.00 25.15	$\mathtt{BLGL}$
MOTA	1017		TYR	140	-11.259	-0.580	38.167	1.00 25.77	BLGL
ATOM	1018	CD2	TYR	140	-9.492	-1.508	36.247	1.00 22.26	BLGL
ATOM	1019		TYR	140	-10.353	-0.457	35.950	1.00 24.44	BLGL
ATOM	1020	CZ	TYR	140	-11.235	0.003	36.911	1.00 25.75	BLGL
ATOM	1021	ОН	TYR	· 140	-12.096	1.036	36.615	1.00 25.22	BLGL
ATOM	1022	Ç	TYR	140	-7.393	-1.468	39.272	1.00 27.76	BLGL
ATOM	1023	0	TYR	140	-7.167	-0.335	38.845	1.00 26.59	BLGL
ATOM	1024	N	GLN	141	-7.828	-1.698	40.508	1.00 29.36	BLGL
MOTA	1025	CA	GLN	141	-8.061	-0.605	41.446	1.00 31.47	BLGL
MOTA	1026	CB	GLN	141	-8.645	-1.134	42.758	1.00 34.45	BLGL
ATOM	1027	CG	GLN	141	-10.105	-1.525	42.664	1.00 44.36	BLGL .
MOTA	1028	CD	GLN	141	-11.015	-0.331	42.408	1.00 49.85	BLGL
ATOM	1029	OE I	GLN	141	-12.161	-0.487	41.957	1.00 52.06	BLGL
MOTA	1030	NE2	GLN	141	-10.515	0.870	42.707	1.00 49.83	BLGL
MOTA	1031	C	GFN	141	-6.782	0.154	41.751	1.00 29.93	BLGL BLGL
ATOM	1032	0	GLN	141	-6.751	1.387	41.698	1.00 28.20	BLGL
MOTA	1033	N	TYR	142	-5.730	-0.593	42.079	1.00 27.46	BLGL
MOTA	1034	CA	AYT	142	-4.445	-0.002	42.413	1.00 25.44	BLGL
MOTA	1035	CB	TYR	142	-3.426	-1.105	42.694	1.00 26.98	BLGL
ATOM	1036	CG	TYR	142	-2.025	-0.585	42.928	1.00 26.89 1.00 25.19	BLGL
MOTA	1037		L TYR	142	-1.752	0.281	43.979	1.00 28.95	BLGL
ATOM	1038		L TYR	142	-0.473		44.189 42.088	1.00 27.59	BLGL
MOTA	1039		2 TYR	142	-0.979	-0.950		1.00 27.33	BLGL
MOTA	1040		2 TYR		0.305	-0.468			BLGL
ATOM	1041	CZ	TYR		0.553	0.390		1.00 32.86	BLGL
MOTA	1042	OH	TYR		1.829	0.862			BLGL
ATOM	1043	C	TYR		-3.922	0.912			BLGL
MOTA	1044	0	TYR		-3.466	2.026			BLGL
ATOM	1045	N	THR		-3.988	0.432			BLGL
ATOM		CA			-3.518 -3.626	1.205			BLGL
ATOM	1047	CB			-3.626	0.397			BLGL
ATOM	1048		1 THR		-3.000	-0.875			BLGL
ATOM	1049		2 THR		~2.948	1.129			BLGL
ATOM	1050		THR		-4.361	2.459			BLGL
MOTA	1051	0	THR		-3.836 -5.673	3.568 2.263			BLGL
ATOM	1052	N	LYS		-5.673 -6.636				BLGL
MOTA	1053				~8.053		_		BLGL
MOTA	1054	CB			-9.167	3.787			BLGL
MOTA	1055	CG	LYS	144	-2.10/	2.707	50.020		

Fig. 4 cont.

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ATOM	1056	CD	LYS	144	-9.391	4.123	37.167	1.00 35.17	BLGL		
MOTA	1057	CE	LYS	144	-10.603	5.033	37.010	1.00 36.95 1.00 37.88	BLGL BLGL		
MOTA	1058	NZ	LYS	144	-11.835	4.435 4.421	37.605 39.748	1.00 37.88	BLGL		
ATOM ATOM	1059 1060	С 0	LYS LYS	144 144	-6.401 -6.322	5.606	39.433	1.00 29.09	BLGL		
ATOM .	1060	N	GLN	145	-6.287	4.010	41.004	1.00 28.65	BLGL		
MOTA	1062	CA	GLN	145	-6.062	4.969	42.075	1.00 31.28	BLGL		
ATOM	1063	CB	GLN	145	-6.116	4.281	43.440	1.00 35.75	BLGL BLGL		
ATOM	1064	CG	GLN	145	-7.463 -8.638	3.632 · 4.586	43.756 43.565	1.00 45.00 1.00 50.27	BLGL		
ATOM ATOM	1065 1066	CD OE1	GLN GLN	145 145	-8.697	5.651	44.189	1.00 53.13	BLGL		
ATOM	1067		GLN	145	-9.580	4.206	42.699	1.00 51.05	BLGL		
ATOM	1068	C	GLN	145	-4.720	5.666	41.905	1.00 30.73	BLGL		
MOTA	1069	0	GLN	145	-4.653	6.895	41.883	1.00 31.69 1.00 28.68	BLGL BLGL		
MOTA	1070	N	SER	146	-3.655	4.880	41.778 41.614	1.00 28.66	BLGL		
MOTA	1071 1072	CA CB	SER SER	146 ' 146	-2.315 -1.326	5.429 4.319	41.276	1.00 26.10	BLGL		
MOTA MOTA	1072	OG	SER	146	-1.175	3.432		1.00 25.05	BLGL		
MOTA	1074	C	SER	146 .	-2.258	6.485	40.529	1.00 26.20	BLGL		
ATOM	1075	0	SER	146	-1.733	7.576	40.739	1.00 24.18	BLGL		
ATOM	1076	N	<b>TE</b> U	147	-2.793	6.148	39.363	1.00 26.95 1.00 28.50	BLGL BLGL		
ATOM	1077	CA	LEU	147	-2.798 -3.399	7.069 6.386	38.240 37.004	1.00 28.30	BLGL		
ATOM ATOM	1078 1079	CB CG	LEU LEU	147 147	-2.403	5.891	35.949	1.00 29.50	BLGL		
ATOM	1080		LEU	147	÷1.214	5.237	36.616	1.00 31.84	BLGL		
MOTA	1081		LEU	147	-3.098	4.918	35.010	1.00 31.26.	. BLGL		
MOTA	1082	С	LEU	147	-3.554	8.352	38.563	1.00 28.49	BLGL		
ATOM	1083	O	LEU	147	-3.059	9.448	38.291	1.00 26.93 1.00 29.43	BLGL BLGL		
MOTA	1084	N	LYS	148	-4.740 -5.520	8.227 9.412	39.156 39.485	1.00 29.43	BLGL		
MOTA MOTA	.1085 1086	CA CB	LYS LYS	148 148	-6.897	9.041	40.039	1.00 35.85	BLGL		
MOTA	1087	CG	LYS	148	-7.879	10.208	39.955	1.00 44.89	BLGL		
MOTA	1088	CD	LYS	148	-9.276	9.854	40.430	1.00 48.80	Brcr		
ATOM	1089	CE	LYS	148	-9.319	9.641	41.939	1.00 53.72	BLGL		
MOTA	1090	NZ	LYS	148	-8.537 -4.772	8.451	42.388 40.488	1.00 55.41 1.00 30.09	BLGL BLGL		
ATOM	1091 1092	0	LYS LYS	148 148	-4.833	11.502	40.400	1.00 30.55	BLGL		
ATOM ATOM	1092	N	ALA	149	-4.063	9.636	41.412	1.00 27.72	BLGL		
ATOM	1094	CA	ALA	149	-3.279	10.352	42.411	1.00 27.90	BLGL		
MOTA	1095	CB	ALA	149	-2.623	9.367	43.368	1.00 26.54	BLGL		
ATOM	1096	С	ALA	149	-2.208	11.196	41.720	1.00 28.02 1.00 27.39	BLGL BLGL		
ATOM	1097	0	ALA MET	149 150	-1.981 -1.547	12.357 10.607	42.075 40.729	1.00 27.66	BLGL		
ATOM ATOM	1098 1099	N CA	MET	150	-0.511	11.319	39.996	1.00 28.87	BLGL		
MOTA	1100	СВ	MET	150	0.228	10.357	39.063	1.00 28.84	Brcr		
ATOM	1101	CG	MET	150	1.084	9.358	39.828	1.00 31.73	BLGL		
MOTA	1102	SD	MET	150	2.122	8.307	38.803	1.00 34.53	BLGL BLGL		
MOTA	1103	CE	MET	150	1.218 -1.101	6.808 12.491	38.827 39.219	1.00 36.46 1.00 28.60	BLGL		
ATOM ATOM	1104 1105	0	MET MET	150 150	-0.518	13.575	39.167	1.00 25.71	BLGL		
ATOM	1106	N	LYS	151	-2.269	12.274	38.626	1.00 30.33	BLGL		
MOTA	1107	CA	LYS	151	-2.939	13.327	37.871	1.00 31.72	BLGL		
MOTA	1108	CB	LYS	151	-4.229	12.793		1.00 32.47	BLGL		
ATOM	1.109	CG	LYS		-4.036	12.005	35.980	1.00 35.00 1.00 38.64	BLGL BLGL		
ATOM	1110	CD	LYS		-3.833 -3.939	12.927 12.159	34.789 33.477	1.00 30.04	BLGL		
mota Mota	1111 1112	CE NZ	LYS		~3.816	13.050	_	1.00 40.80	BLGL		
ATOM	1113	C	LYS		-3.261	14.501	38.787	1.00 31.68	BLGL		
ATOM	1114	0	LYS	151	-3.008	15.655			BLGL		
ATOM	1115	N	ALA		-3.823	14.199		1.00 31.23	BLGL		
ATOM	1116	CA	ALA		-4.176	15.228		1.00 30.30 1.00 29.61	BLGL BLGL		
ATOM	1117 1118	CB	ALA ALA		-4.759 -2.952	14.590 16.057			BLGL		
MOTA MOTA	1118	C	ALA		-3.066	17.247		1.00 30.53	BLGL		
ATOM	1120	N	ALA		-1.783	15.425	41.272	1.00 29.04	BLGL		
ATOM	1121	CA	ALA		-0.543	16.124	41.596	1.00 29.10	BLGL		
						_					

Fig. 4 cont.

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MOTA	1122	CB	ALA	153	0.517	15.134	42.032	1.00 30.13	BLGL		
ATOM	1123	С	ALA	153		16.910	40.391	1.00 29.10 1.00 29.45	BLGL BLGL		
ATOM	1124	0	ALA	153	0.990 -0.824	17.561 16.835	39.310	1.00 28.65	BLGL		
MOTA	1125	N CA -	GLY GLY	154 154	-0.482	17.557	38.101	1.00 26.76	BLGL		
ATOM ATOM	1126 1127	C	GLY	154	0.711	17.017	37.340	1.00 26.93	. BLGL		
ATOM	1128	ō	GLY	154	1.406	17.770	36.661	1.00 25.28	BLGL		
MOTA	1129	N	ILE	155	0.948	15.713	37.444	1.00 27.10	BLGL		
MOTA	1130	CA	ILE	155	2.064	15.080	36.745 37.496	1.00 25.61 1.00 24.73	BLGL BLGL		
ATOM	1131	CB	ILE	155 155	2.532 3.661	13.809 13.118	36.724	1.00 23.73	BLGL		
ATOM ATOM	1132 1133		IPE	155	2.985	14.196	38.907	1.00 22.31	BLGL		
MOTA	1134		ILE	155	3.188	13.018	39.842	1.00 21.74	BLGL		
MOTA	1135	С	ILE	155	1.672	14,723	35.306	1.00 24.09	BLGL		
MOTA	1136	0	ILE	155	0.568	14.240	35.056	1.00 25.01 1.00 21.70	BLGL BLGL		
ATOM	1137	N	ASP	156	2.581 2.354	14.975 14.695	34.369 32.959	1.00 21.70	BLGL		
ATOM ATOM	1138 1139	CA CB	ASP ASP	156 156	3.172	15.657	32.089	1.00 26.46	BLGL		
ATOM	1140	CG	ASP	156	2.889	15.486	30.602	1.00 30.77	BLGL		
ATOM	1141		ASP	156	3.579	16.140	29.792	1.00 33.81	BLGL		
MOTA	1142	OD2	ASP	156	1.976	14.706	30.239	1.00 32.30	BLGL BLGL		
MOTA	1143	C	ASP	156	2.757	13.261 12.986	32.644 32.319	1.00 23.58 1.00 26.10	BLGL		
MOTA	1144	0	asp ile	156 157	3.904 1.805	12.348	32.750	1.00 22.55	BLGL		
ATOM ATOM	1145 1146	N CA	ILE	.157	2.062	10.945	32,484	1.00 21.98	BLGL		
ATOM	1147	CB	ILE	157	1.070	10.058	33.254	1.00 22.84	BLGL		
ATOM	1148	CG2	•	157	1.368	8.595	32.990	1.00 18.93	BLGL BLGL		
MOTA	1149	CG1		157	1.137	10.385 9.922	34.744 35.514	1.00 23.81 1.00 26.52	BLGL		
ATOM	1150		ILE	157 157	-0.082 1.894	10.675	30.997	1.00 20.48	. BLGL		
MOTA MOTA	1151 1152	С 0	ILE	157	0.819	10.885	30.443	1.00 22.51	BLGL		
ATOM	1153		GLY	158	2.950	10.207	30.349	1.00 18.57	BLGL		
ATOM	1154	CA	GLY	158	2.847	9.927	28.935	1.00 16.55	BLGL		
ATOM	1155	C	GLY	158	2.758	8.445	28.632	1.00 17.26 1.00 17.93	BLGL BLGL		
ATOM	1156	0	GLY	158 159	2.227 3.245	B.042 7.622	27.599 29.550	1.00 17.93	BLGL		
atom atom	1157 1158	N CA	MET MET	159	3.243	6.186	29.322	1.00 19.00	BLGL		
ATOM	1159	CB	MET	159	4.559	5.834	28.588	1.00 17.91	BLGL		
ATOM	1160	CG	MET	159	4.563	4.506	27.872	1.00 24.08	BLGL		
MOTA	1161	SD	MET	159	6.139	4.167	27.000	1.00 30.17 1.00 26.74	BLGL BLGL		
ATOM	1162	CE	MET	159 159	6.095 3.156	5.442 5.395	25.740 30.630	1.00 28.74	BLGL		
ATOM ATOM	1163 1164	C	MET MET	159	3.573	5.855	31.696	1.00 16.99	BLGL		
MOTA	1165	N	VAL	160	2.579	4.204	30.543	1.00 18.21	BLGL		
ATOM	1166	CA	VAL	160	2.450	.3.345	31.707	1.00 17.42	BLGL		
ATOM	1167	СB	VAL	160	1.002	3.285	32.245	1.00 17.75	BLGL BLGL		
ATOM	1168		LVAL	160	0.920 0.570	2.287 4.654	33.384 32.739	1.00 16.21 1.00 18.60	BLGL		
MOTA	1169 1170		LAV S	160 160	2.891	1.944	31.332	1.00 17.12	BLGL		
MOTA MOTA	1171	C	VAL	160	2.516	1.406	_	1.00 17.78	BLGL		
ATOM	1172	N	GLN	161	3.704	1.360	32.192	1.00 17.31	BLGL		
ATOM	1173	CA	GLN	161	4.211	0.028	31.963	1.00 17.58	BLGL		
MOTA	1174	CB	GLN	161	5.709	0.018	32.272 31.826	1.00 17.55 1.00 16.31	BLGL BLGL		
MOTA	1175 1176		GLN GLN	161 161	6.446 7.935	-1.213 -1.106			BLGL		
MOTA MOTA	1177		1 GLN	161	8.570			1.00 17.05	BLGL		
ATOM	1178		2 GLN	161	8.508	-2.114		1.00 12.70	BLGL		
MOTA	1179		GLN	161	3.439		_		BLGL		
ATOM	1180		GLN	161	3.455				BLGL BLGL		
ATOM	1181		VAL	162	2.736				BLGL		
ATOM	1182			162 162	1.975 0.648	_			BLGL		
MOTA MOTA	1183 1184		VAL 1 VAL	162	-0.143				BLGL		
ATOM	1185		2 VAL	162	-0.176		32.213	1.00 12.73	BLGL		
ATOM	1186		VAL		2.840			1.00 15.01	BLGL		
ATOM	1187		VAL	162	2.763	-5.046	32.691	1.00 15.57	BLGL		

Fig. 4 cont.

### 144/174 1.00 13.93 BLGL -3.965 34.444 3.674 1188 GLY 163 ATOM N -5.062 34.765 1.00 16.33 BLGL 4.568 ATOM 1189 CA GLY 163 1.00 17.03 BLGL 34.350 6.001 -4.755163 1190 GLY MOTA C -3.875 33.521 1.00 17.31 BLGL 6.239 163 ATOM 1191 0 GLY BLGL 34.917 1.00 17.42 -5.485 ASN 164 6.958 ATOM 1192 N 1.00 16.23 BLGL -5.27434.628 164 8.374 ATOM 1193 CA ASN 1.00 13.47 BLGL -4.629 35.845 164 9.035 1194 ASN ATOM CB -4.117 1.00 11.45 BLGL 35.556 ASN 164 10.413 ATOM 1195 CG 1.00 13.59 BLGL -3.019 35.026 10.581 1196 OD1 ASN 164 ATOM -4.912 35.889 1.00 11.01 BLGL 11.416 1197 ND2 ASN 164 ATOM 1.00 17.48 BLGL 9.051 -6.61434.315 ASN 164 ATOM 1198 C 1.00 19.59 BLGL -7.490 35.175 9.131 164 ATOM 1199 0 ASN 33.085 1.00 17.58 BLGL 9.537 -6.765 165 MOTA 1200 N GLU -7.998 BLGL 32.643 1.00 17.54 165 10.197 ATOM 1201 CA GLU 1.00 16.33 BLGL -8.093 33.244 165 11.605 GLU MOTA 1202 CB BLGL 32.940 1.00 17.40 -6.875 165 12.467 ATOM 1203 CG GLU BLGL 13.938 ~7.095 33.223 1.00 17.97 165 GLU ATOM 1204 · CD BLGL 1.00 20.07 34.236 165 14.260 -7.739 ATOM 1205 OE1 GLU 14.783 -6.613 32.442 1.00 15.79 BLGL 165 OE2 GLU ATOM' 1206 1.00 16.57 BLGL -9.248 32.982 1207 С GLU 165 9.372 MOTA 33.534 1.00 14.22 BLGL 9.875 -10.221 GLU 165 MOTA 1208 0 1.00 16.92 BLGL 32.618 B.094 -9.196 ATOM 1209 N THR 166 BLGL' 166 7.146 -10.267 32.860 1.00 15.12 THR 1210 CÀ ATOM BLGL 1.00 17.38 32.782 5.723 -9.713MOTA 1211 CB THR 166 BLGL 1.00 16.95 166 5.514 -9.130 31.490 OG1 THR 1212 MOTA 1.00 17.63 BLGL -8.629 33.850 1213 CG2 THR 166 5.511 MOTA 1.00 15.92 BLGL . 7.304 -11.411 166 31.860 MOTA 1214 С THR 6.380 -11.741 31.131 1.00 13.18 BLGL THR 166 MOTA 1215 0 BLGL 8.488 -12.013 31.835 1.00 18.90 167 ATOM 1216 ASN N 1.00 19.84 1.00 19.56 30.933 BLGL 167 167 ASN 8.775 -13.122 ATOM 1217 CA BLGL 10.277 -13.399 30.885 1218 CB ASN ATOM 1.00 19.68 11.014 -12.455 29.974 BLGL 1219 ASN 167 MOTA CG 1.00 21.70 BLGL 10.597 -11.320 29.774 ATOM 1220 OD1 ASN 167 1.00 19.90 1.00 20.80 BLGL 12.132 -12.912 29.429 1221 ND2 ASN 167 MOTA BLGL 8.074 -14.397 31.343 ASN 167 MOTA 1222 C 7.670 -15.175 1.00 22.87 BLGL 30.489 MOTA 1223 O ASN 167 1.00 22.03 BLGL 7.936 -14.615 32.647 1224 GLY 168 ATOM N 7.302 -15.833 33.114 1.00 24.61 BLGL 168 ATOM 1225 ÇA GLY 1.00 26.99 BLGL 1226 С GLY 168 6.216 -15.699 34.164 ATOM 5.663 -16.702 1.00 28.98 BLGL 34.620 168 ATOM 1227 0 GLY 1.00 26.63 34.562 BLGL 5.898 -14.478 1228. GLY 169 ATOM N 1.00 25.86 BLGL 4.865 -14.319 35.558 ATOM 1229 CA GLY 169 1.00 27.02 BLGL 4.516 -12.878 35.831 GLY 169 1230 С MOTA 5.166 -11.959 1.00 28.44 BLGL 35.334 1231 GLY 169 ATOM 0 1.00 26.37 BLGL 3.467 -12.691 LEU 170 36.622 1232 ATOM N 37.005 1.00 23.73 BLGL 2.996 -11.371 ATOM 1233 CA LEU 170 1.00 20.57 BLGL 2.164 -10.751 35.875 1234 LEU 170 ATOM CB 1.00 21.09 BLGL 1.474 -9.415 36.185 170 MOTA 1235 CG LEU BLGL 36.723 1.00 21.42 170 2.470 -8.395 1236 CD1 LEU ATOM 1.00 20.49 BLGL 0.811 -8.894 34.934 170 CD2 LEU MOTA 1237 1.00 23.90 BLGL 1238 LEU 170 2.158 -11.504 38.272 MOTA C 1.222 -12.305 1.00 22.71 BLGL 38.326 170 ATOM 1239 0 LEU BLGL 39.292 1.00 23.01 1240 ALA 171 2.522 -10.731 N ATOM 40.567 1.00 22.14 BLGL 1.816 -10.724 ALA 171 ATOM 1241 CA 1.00 22.04 BLGL ATOM 1242 CB ALA 171 0.544 -9.911 40.433 BLGL 1.488 -12.114 41.109 1.00 23.55 171 ATOM 1243 С ALA BLGL 41.512 1.00 23.66 171 0.354 -12.382 MOTA 1244 0 ALA 2.479 -12.996 41.122 1.00 22.96 BLGL ATOM 1245 N GLY 172 1.00 25.97 BLGL 2.259 -14.337 41.632 ATOM 1246 CA GLY 172 1.592 -15.299 40.666 1.00 27.36 BLGL 172 ATOM 1247 С GLY 1.00 27.94 BLGL 1.412 -16.474 40.980 ATOM 1248 a GLY 172 1.00 28.30 BLGL 1.225 -14.808 39.490 173 ATOM 1249 N GLU 1.00 29.90 BLGL 0.584 -15.643 38,487 ATOM 1250 CA GLU 173 1.00 30.87 BLGL -0.540 -14.858 173 37.815 MOTA 1251 CB GLU 1.00 33.63 BLGL 173 -1.888 -15.557 37.824 ATOM 1252 CG GLU

Fig. 4 cont.

39,208

-2.308 -16.014

GLU

CD

ATOM

1253

173

1.00 34.41

BLCL

							<i>)</i>       <del>   </del>					
MOTA	1254	OE1	GLU	173		-2.334 - 1	L5.181	40.139		34.20		3LGL
ATOM	1255	OE2	GLU	173		-2.618 -3	17.214	39.359		34.57		BLGL
ATOM	1256		GLU	173		1.619 -	16.084	37.450	1.00	30.77	· 1	<b>3LGL</b>
ATOM	1257		GLU	173		2,481 -1	15.302	37.053	1.00	31.69	1	BLGL
ATOM	1258		THR	174		1.539 -3		37.017	1.00	30.71	1	BLGL
MOTA	1259		THR	174		2.484 -		36.038	1.00	30.81	3	BLGL
			THR	174		3.366 -		36.661	1.00	30.70	1	BLGL
ATOM	1260	OG1		174		2.533 -		37.167	1.00	33.92		BLGL
ATOM	1261			174		4.201 -		37.792		29.44		BLGL
ATOM	1262	CG2				1.801 -		34.792		31.23		BLGL
ATOM	1263	С	THR	174				33.857		31.14		BLGL
MOTA	1264	0	THR	174		2.470 -				31.31		BLGL
MOTA	1265	N	ASP	175		0.473 -		34.779				BLGL
MOTA	1266	CA	ASP	175		-0.276 -		33.640		31.53		
MOTA	1267	CB	asp	175		-1.565 -		34.120		35.17		BLGL
MOTA	1268	CG	ASP	175	٠,	-2.447 -	20.030	32.972		38.71		BLGL
MOTA	1269	OD1	ASP .	175.		-1.925 -	20.654	32.023		39.79		BLGL
MOTA	1270	OD2	ASP	175		-3.665 -	19.758	33.022		42.47		BLGL
ATOM	1271	С	ASP	175	•	-0.605 -	17.796	32.674	1.00	30.63		BLGL
MOTA	1272	ο .		175		-1.363 -	16.890	33.016	1.00	30.64		BLGL
ATOM	1273	N .	TRP	.176		-0.055 -	17.861	31.463	1.00	27.62		BLGL
ATOM	1274	CA	TRP	176		-0.281 -		30.480	1.00	27.93		BLGL
ATOM	1275	CB	TRP	176		0.403 -		29.157	1.00	24.63		BLGL
ATOM	1276	CG	TRP	176		1.882 -		29.193		26.55		BLGL
	1277		TRP	176		2.557		28.966		27.36		BLGL
MOTA				176	•	3.940 -		29.148		27.27		BLGL
ATOM	1278		TRP	176		2.128		28.625		27.01		BLGL
ATOM	1279		TRP			2.855 -		29.498		26.56		BLGL
ATOM.	1280		TRP	176		4.094 -		29.473		26.37		BLGL
MOTA	1281		TRP	176				-		25.56		BLGL
MOTA	1282		TRP	176		4.899 -		29.004				BLGL
MOTA	1283		TRP	176		3.085 -		28.482		25.94		
MOTA	1284			176		4.453 -		28.671		25.57		BLGL
MOTA	1285	С	TRP	-		-1.739 -		30.234		29.80		BLGL
ATOM	1286	0	TRP	176		-2.033 -	_	29.857		30.42		BLGL
MOTA	1287	И	ALA	177		-2.656 -		30.441		31.37		BLGL
MOTA	1288	CA	ALA	177		-4.073 -	-17.077	30.249		30.31		BLGL
ATOM	1289	CB	ALA	177		-4.889 -	-18.354	30.339		30.40		BLGL
ATOM	1290	Ċ	. ALA	177		-4.500 -	16.104	31.342	1.00	31.32		BLGL
MOTA	1291	0	ALA	177		-5.199 -	-15.124	31.085	1.00	31.10		BLGL
ATCM	1292	N	LYS	178		-4.070 -	-16.379	32.569	1.00	30.35		BLGL
ATOM	1293	CA	LYS	178		-4.401 -	-15.507	33.680	1.00	31.58		BLGL
ATOM	1294	CB	LYS	178		-4.181 -		35.008	1.00	33.69		BLGL
ATOM	1295	CG	LYS	178		-5.114 -		35.234	1.00	37.35		BLGL
ATOM	1296	CD	LYS	178		-4.994 -		36.664	1.00	43.39		BLGL
MOTA	1297	CE	LYS	178		-5.780 -		36,897		45.38		BLGL
ATOM	1298	NZ	LYS	178		-5.125 -		36.252		47.94		BLGL
ATOM	1299	C	LYS	178		-3.568 -		33.637		30.97		BLGL
	1300	Ö	LYS	178		-4.040 -		34.043		31.65		BLGL
ATOM		N	MET	179	•	-2.333 -		33.149		29.06		BLGL
ATOM	1301					-1.485		33.062		26.50		BLGL
ATOM	1302	CA	MET	179		-0.110 -		32.521		27.08		BLGL
MOTA	1303	CB	MET	179			-14.179	33.507		29.22		BLGL
ATOM	1304	CG	MET	179						32.04		BLGL
ATOM	1305	SD	MET	179			-14.378	32.801				BLGL
ATOM	1306	ÇE	MET	179			-16.100	32.529		37.19		
MOTA	1307	C	MET	179		-2.122		32.141		0 25.11		BLGL
MOTA	1308	0	Met	179		-2.206		32.478		0 24.38		BLGL
MOTA	1309	N	SER	180		-2.566 ·		30,977		0 23.38		BLGL
ATOM	1310	CA	SER	180		-3.199	-11.707	29.985		0 23.70		BLGL
MOTA	1311	CB	SER	180		-3.725		28.812		0 23.12		BLGL
MOTA	1312	OG	SER	180		-2.691	-13.297	28.223		0 23.86		BLGL
ATOM	1313	С	SER			-4.348	-10.933	30.605	1.0	0 24.08		BLGL
ATOM	1314	0	SER			-4.552	-9.756	30.313	1.0	0 23.86		BLGL.
ATOM	1315	N	GLN			-5.101		31.467	1.0	0 25.04		BLGL
ATOM	1316	CA	GLN			-6.226		32.129		0 27.04		BLGL
ATOM	1317	CB	GLN	181		-7.064		32.864	1.0	0 29.17		BLGL
ATOM	1318	CG	GLN			-7.820				0 33.08	•	BLGL
Atom	1319	CD	GLN			-8.761				0 35.97		BLGL
WI OLI	1313	CD	OTI1A	TOT		0.701		J2.07J				

Fig. 4 cont.

146/174 BLGL -8.558 -15.077 32.724 1.00 36.76 OE1 GLN 181 MOTA 1320 33.269 1.00 37.03 BLGL -9.801 -13.280 181 NE2 GLN ATOM 1321 BLGL 1.00 27.11 33.091 -5.774 -9.874 181 1322 C GLN ATOM 33.252 1.00 28.46 BLGL -6.459 -8.864 181 GLN ATOM 1323 0 BLGL 33.737 1.00 26.80 -4.628 -10.080 LEU 182 1324 N ATOM BLGL 1.00 25.48 34.655 -4.086 -9.081 LEU 182 MOTA 1325 CA BLGL -9.665 1.00 25.40 35.472 -2.932 LEU 182 1326 CB ATOM 1.00 27.62 BLGL -3.296 -10.736 36.504 182 LEU ATOM 1327 CG BLGL 1.00 27.60 37.156 -2.035 -11.268 132B CD1 LEU 182 ATOM 1.00 26.92 BLGL 37.556 -4.229 -10.149 182 MOTA 1329 CD2 LEU BLGL 33.823 1.00 24.10 -7.899 182 -3.591 1330 LEU MOTA C 1.00 23.49 BLGL -3.739 -6.74034.211 182 LEU MOTA 1331 ٥ BLGL 1.00 21.91 32.675 -B.211 183 -3.000 1332 N PHE MOTA 1.00 22.28 BLGL -7.187 31.770 -2.512 183 PHE **ATOM** 1333 CA 1.00 21.38 BLGL 30.528 ~7.826 1334 CB PHE 183 -1.888 ATOM 1.00 20.19 BLGL 183 -0.500 -8.347 30.737 PHE ATOM 1335 CG 30.042 1.00 20.38 BLGL -9.469 -0.064 1336 CD1 PHE 183 ATOM 1.00 22.77 BLGL -7.70431.597 0.385 PHE 183 MOTA 1337 CD2 30.192 1,00 20.30 BLGL ~9.953 -8.174 MOTA 1338 CE1 PHE 183 1.236 1.00 24.59 BLGL 1.693 31.761 183 1339 CE2 PHE ATOM 1.00 23.28 BLGL 31.054 -9.305 183 2.120 ATOM 1340 CZPHE BLGL 1.00 22.44 -3.668 -6.28331.348 ATOM 1341 С PHE 183 31.384 1.00 22.23 BLGL -5.059 -3.548 183 MOTA 1342 0 PHE 1.00 22.00 BLGL 184 -4.792 -6.881 30.954 ASN MOTA 1343 N BLGL -6.087 30.533 1.00 20.53 184 -5.939ATOM 1344 CA ASN 1.00 20.92 BLGL -6.96429.895 184 -7.012 ASN ATOM 1345 CB -7.345 28.474 1.00 21.95 BLGL -6.677 ASN 184 AŤOM 1346 CG 1.00 24.93 BLGL -6.162 -6.535 27.708 OD1 ASN 184 ATOM 1347 1.00 26.02 BLGL -6.983 -8.579 28.108 ASN 184 ATOM 1348 ND2 1.00 17.99 BLGL 31.679 -6.538 -5.293 184 1349 C ASN ATOM -4.199 31.474 BLGL 1.00 18.30 -7.053 MOTA 1350 0 ASN 184 1.00 16.83 BLGL -6.458-5.841 32.884 185 1351 N ALA MOTA BLGL 1.00 18.27 -6.976-5.163 34.066 1352 ALA 185 MOTA CA 1.00 16.14 BLGL 35.294 -6.815-6.048185 ATOM 1353 CB ALA -3.857 1.00 18.87 BLGL 34.261 -6.21,5 ALA 185 ATOM 1354 C 1.00 17.89 BLGL -6.812 -2.79534.422 185 MOTA 0 ALA 1355 BLGL 1.00 20.07 -3.945 34.244 1356 N GLY 186 -4.888 ATOM 1.00 19.75 BLGL -2.756 34.409 -4.073 186 GLY ATOM 1357 CA -1.834 BLGL -4.273 33.226 1.00 19.07 1358 GLY 186 MOTA 1.00 20.22 BLGL -0.620 -4.367 33.373 1359 O GLY 186 MOTA BLGL 32.042 1.00 18.72 -2.424 -4.345 1360 N SER 187 MOTA 1.00 18.78 BLGL -4.534 -1.664 30.819 187 CA SER ATOM 1361 BLGL 1.00 19.99 -2.618 29:627 -4.570 ATOM 1362 CB SER 187 1.00 22.89 BLGL -4.606 -1.903 28.409 SER 187 OG MOTA 1363 1.00 20.30 BLGL -0.877 30.897 -5.840 MOTA 1364 С SER 187 1.00 20.23 BLGL 187 -5.879 0.311 30.582 SER 1365 O MOTA BLGL -6.903 -1.554 31.325 1.00 19.43 188 MOTA 1366 N GLN 1.00 20.10 BLGL 31.465 GLN 188 -8.233 -0.960 CA MOTA 1367 BLGL 32.093 1.00 21.27 -1.990-9.192 MOTA 1368 CB GLN 188 1.00 24.00 BLGL 32.439 GLN 188 -10.592 -1.480CG MOTA 1369 -11.358 -0.97331.228 1.00 29.54 BLGL 188 1370 CD GLN MOTA 1.00 33.67 BLGL 30.242 OE1 GLN 188 -11.546 -1.6951371 ATOM BLGL -11.808 0.274 31.295 1.00 28.21 ATOM 1372 NE2 GLN 188 BLGL 1.00 20.12 32.322 -8.191 0.303 1373 GLN 188 C ATOM BLGL 188 -8.779 1.322 31.984 1.00 19.92 1374 0 GLN MOTA 1.00 20.06 BLGL 33.442 -7.4930.227 **ATOM** 1375 N ALA 189 BLGL 34.329 1.00 19.56 -7.383 1.366 189 ATOM 1376 CA ALA 1.00 18.86 BLGL 35.563 -6.587 0.982 1377 ALA 189 ATOM CB BLGL 2.546 1.00 19.66 -6.728 33.626 ATOM 1378 C ALA 189 1.00 20.48 BLGL -7.150 3.681 33.805 ALA 189 1379 0 MOTA 1.00 19.85 BLGL -5.697 2.273 32.831 VAL 190 ATOM 1380 N BLGL 1.00 21.68 -4.984 3.324 32.108 VAL 190 ATOM 1381 CA BLGL 1.00 21.13 31.378 -3.717 2.755 VAL 190 MOTA 1382 CB 1.00 17.97 BLGL -2.955 3.875 30.675 CG1 VAL 190 ATOM 1383 BLGL 1.00 18.02 32.376 CG2 VAL 190 -2.809 2.069 ATOM 1384 1.00 22.56 BLGL 31.087 -5.922 3.966 VAL 190 C MOTA 1385

Fig. 4 cont.

	147/174										
ATOM	1386	0	VAL	190	-6.041	5.190	31.007	1.00 21.59	BLGL		
ATOM	1387		ARG	191	-6.590	3.122	30.311	1.00 24.93	BLGL		
MOTA	1388	CA	ARG	191	-7.528	3.577	29.297	1.00 24.90 1.00 22.96	BLGL BLGL		
MOTA	1389	CB	ARG	191	-8.199	2.375	28.640 27.236	1.00 25.30	BLGL		
ATOM	1390	CG	ARG ARG	191 191	-7.687 -6.416	2.059 1.230	27.230	1.00 24.11	BLGL		
ATOM ATOM	1391 1392	CD NE	ARG	191	-5.369	1.936	26.503	1.00 24.46	BLGL		
ATOM	1393	CZ	ARG	191	-4.581	1.653	25.474	1.00 21.34	BLGL		
ATOM	1394	NH1		191	-3.733	2.613	25.208	1.00 22.37	BLGL		
MOTA	1395	NH2	ARG	191	-4.584	0.551	24.731	1.00 21.45	BLGL		
ATOM	1396	С	ARG	191	-8.590	4.492	29.892 29.334	1.00 25.14 1.00 27.85	BLGL BLGL		
MOTA	1397	0	ARG	191 192	-8.904 -9.145	5.535 4.098	31.026	1.00 25.90	BLGL		
ATOM ATOM	1398 1399	N CA	GLU GLU.	192	-10.170	4.895	31.683	1.00 28.14	BLGL		
ATOM	1400	CB	GLU	192	-10.761	4.129	32.865	1.00 28.90	BLGL		
ATOM	1401	CG	GLU	192	-11.776	3.079	32.494	1.00 31.91	BLGL		
MOTA	1402	CD	GLU	192	-12.200	2.266	33.697	1.00 32.43	BLGL		
MOTA	1403		GLU		-12.359	2.874	34.772	1.00 28.80 1.00 34.08	. BLGL BLGL		
ATOM	1404	OE2	GLU	192	-12.378 -9.630	1.033 6.223	33.569 32.190	1.00 34.03	BLGL		
ATOM ATOM	1405 1406	С 0	GLU	192 192	-10.352	7.219	32.278	1.00 31.92	BLGL		
ATOM	1407	N	THR	193	-8.355	6.237	32.541	1.00 27.87	BLGL		
ATOM	1408	CA	THR	193	-7.741	7.445	33.064	1.00 26.29	BLGL		
ATOM	1409	CB	THR	193	-6.416	7.098	33.780	1.00 25.98	· BLGL		
MOTA	1410		THR	193	-6.697	6.231	34.884	1.00 27.07 1.00 24.23	B <b>L</b> GL B <b>L</b> GL		
ATOM	1411		THR	193	-5.725	8.350 8.500	34.296 31.990	1.00 24.23	BLGL		
MOTA	1412 1413	C O	THR THR	193 193	-7.488 -7.827	9.666	32.160	1.00 22.00	BLGL		
MOTA MOTA	1413	N	ASP	194	-6.909	8.084	30.872	1.00 27.05	BLGL		
MOTA	1415	CA	ASP	194	-6.585	9.020	29.810	1.00 27.87	BLGL		
ATOM	1416	CB	ASP	194	-5.396	9.870	30.271	1.00 29.53	BLGL		
ATOM	1417	CG	ASP	194	-4.956	10.881	29.243	1.00 32.75 1.00 34.57	BLGL BLGL		
MOTA	1418		ASP	194	-4.131	11.746 10.816	29.606 28.081	1.00 34.57	BLGL		
MOTA	1419 1420	C C	ASP ASP	194 194	-5.418 -6.245	8.249	28.546	1.00 27.55	BLGL		
MOTA MOTA	1421	0	ASP	194	-5.389	7.368	28.565	1.00 29.57	BLGL		
ATOM	1422	N	SER	195	-6.917	8.580	27.449	1.00 27.67	BLGL		
MOTA	1423	CA	SER	195	-6.690	7.903	26.169	1.00 30.14	BLGL		
MOTA	1424	СВ	SER	195	-7.748	8.333	25.154	1.00 31.04 1.00 38.90	BLGL BLGL		
ATOM	1425	OG	SER	· 195	-9.041 -5.314	7.986 8.137	25.608 25.553	1.00 29.28	BLGL		
ATOM ATOM	1426 1427	С 0	SER SER	195 _. 195	-4.830	7.319	24.773		BLGL		
ATOM	1428	N	ASN	196	-4.690	9.255	25.903	1.00 30.46	BLGL		
ATOM	1429	CA	ASN	196	-3.387	9.600	25.358	1.00 32.52	BLGL		
MOTA	1430	СВ	ASN	196	-3.147	11.097	25.514	1.00 38.65	BLGL		
ATOM	1431	CG	ASN	196	-4.246	11.919	24.892 23.672	1.00 45.74 1.00 47.81	BLGL BLGL		
MOTA	1432		ASN ASN	196 196	-4.436 -4.996	11.902 12.637	25.729	1.00 49.19	BLGL		
ATOM ATOM	1433 1434	C	ASN		-2.232	8.838	25.981	1.00 30.86	BLGL		
ATOM	1435	ō	ASN		-1.141	8.779	25.411	1.00 31.65	BLGL		
MOTA	1436	N	ITE		-2.459	8.260	27.153	1.00 28.33	BLGL		
ATOM	1437	CA	ILE		-1.403	. 7.517	27.816		BLGL		
ATOM	1438	CB	ILE		-1.771	7.224	29.282 29.919		BLGL BLGL		
MOTA	1439		ILE		-0.720 -1.873	6.335 8.542			BLGL		
ATOM ATOM	1440 1441		. ILE		-2.239	8.380			BLGL		
ATOM	1442	Č.	ILE		-1.149	6.222		1.00 23.64	BLGL		
ATOM	1443	ō	ILE	197	-2.081	5.487			BLGL		
ATOM	1444	N	LEU		0.116	5.962	26.754		BLGL		
ATOM	1445	CA	LEU		0.483	4.751			BLGL BLGL		
MOTA	1446	CB	LEU		1.787 1.683	4.962 5.885			BLGL		
ATOM	1447 1448	CG CD1	LEU LEU		3.062	6.252			BLGL		
MOTA MOTA	1448		LEU		0.881	5.188			BLGL		
ATOM	1450	C	LEU		0.653	3.605		1.00 21.75	BLGL		
ATOM	1451	O	LEU		1.250	3.776	28.073	1.00 23.44	BLGL		
					Control of	4	4	•			

Fig. 4 cont.

148/174 2.441 26.666 1.00 20.49 BLGL VAL 199 0.114 MOTA 1452 N 199 0.244 1.266 27.516 1.00 19.26 BLGL 1453 CA VAL ATOM 27.555 1.00 19.98 BLGL 199 -1.040 0.450 ATOM 1454 CB VAL 199 -0.816 -0.815 28.364 1.00 19.20 BLGL VAL MOTA 1455 CG1 28.149 1.00 21.20 BLGL 199 -2.1481.282 ATOM 1456 CG2 VAL 0.376 26.979 1.00 18.65 BLGL VAL 199 1.352 MOTA 1457 C 1.00 16.57 199 1.329 -0.029 25.818 BLGL ATOM 1458 0 VAL 0.061 27.839 1.00 17.36 BLGL MOTA 1459 N ALA 200 2.314 3.436 -0.760 27.432 1.00 17.13 BLGL ATOM 1460 CA ALA 200 27.427 0.087 1.00 15.68 BLGL 200 4.701 ATOM 1461 CB ALA -1.991 -1.960 1.00 16.72 ATOM 28.299 BLGL 1462 C ALA 200 3.645 1.00 15.94 BLGL 3.403 29.501 ATOM 1463 0 ALA 200 4.079 -3.077 27.661 1.00 17.11 BLGL ATOM 1464 LEU 201 N 1.00 17.16 BLGL ATOM 1465 .CA LEU 201 4.390 -4.332 28.339 -5.502 -5.388 3.638 27.706 1.00 17.16 BLGL ATOM 1466 CB LEU 201 1.00 17.50 BLGL 27.753 ATOM 1467 CG LEU 201 2.114 ATOM 1468 CD1 LEU 201 1.497 -6.671 27.236 1.00 20.85 BLGL. 1.00 19.12 BLGL -5.132 29.172 MOTA 1469 CD2 LEU 201. 1.654 5.907 -4.497 28.186 1.00 17.78 BLGL ATOM 1470 С LEU 201 -4.279 1.00 17.49 6.465 27.111 BLGL ATOM 1471 0 LEU 201 1472 6.568 -4.874 29.272 1.00 18.05 BLGL ATOM HIS 202 N -4.981 1.00 17.54 BLGL 8.018 29.294 ATOM 1473 202 CA HIS MOTA 1474 ĊВ HIS 202 8.519 -4.129 30.460 1.00 17.68 BLGL -4.110 1.00 19.94 BLGL 10.002 30.616 ATOM 1475 HIS CG 202 MOTA 1476. CD2 HIS 202 10.998 -4.372 29.741 .1.00 20.39 BLGL ND1 HIS 202 10.613 -3.77331.805 1.00 21.65 BLGL ATOM 1477 MOTA 1.00 22.99 1478 CE1 HIS 202 11,922 -3.831 31.655 BLGL NEZ HIS 12.183 -4.193 30.411 1.00 23.44 BLGL 1479 ATOM. 202 ATOM 1480 202 8.569 -6.400 29.402 1.00 18.30 BLGL C HIS 202 8.272 -7.122 30.354 1.00 18.51 . BLGL ATOM 1481 0 HIS ATOM 1482 PHE 203 9.386 -6.790 28.429 1.00 16.01 BLGL N MOTA 1483 CA PHE 9.989 -8.114 28.431 1.00 16.62 BLGL 203 ATOM 1484 PHE 203 9.398 -8,963 27.316 1.00 13.11 BLGL CB ATOM 1485 CG PHE 203 7.912 -9.055 27.375 1.00 17.34 BLGL ATOM 1486 CD1 PHE 203 7.116 -8.119 26.724 1.00 17.15 BLGL 1.00 15.95 MOTA 1487 CD2 PHE 203 7.299 -10.037 28.144 BLGL ATOM 1488 CE1 PHE 203 5.738 -8.158 26.840 1.00 16.32 BLGL 1.00 16.04 ATOM 1489 CE2 PHE 203 5.925 -10.083 28.266 BLGL 1.00 18.54 ATOM 1490 CZ PHE 203 5.141 -9.14027.612 BLGL 1,491 ATOM 203 11.504 -8.033 28.274 1.00 19.65 BLGL С PHE 12.051 -6.987 1.00 21.99 BLGL ATOM 1492 0 PHE 203 27.910 1.00 17.81 1.00 18.21 MOTA 1493 N THR 204 12.188 -9.13528.552 BLGL BLGL ATOM 1494 CA THR 204 13.634 ~9.133 28,426 14.314 1.00 17.19 ATOM 1495 ÇВ 204 -8.849 29.798 BLGL THR 15.726 -8.736 1.00 14.37 BLGL ATOM 1496 OG1 THR 204 29.611 MOTA 1497 CG2 THR 204 14.006 -9.951 30.809 1.00 13.65 BLGL 1.00 18.61 ATOM 1498 С THR 204 14.161 -10.428 27.809 BLGL 13.394 -11.352 MOTA 1499 O THR 204 27.534 1.00 16,21 BLGL MOTA 1500 Ŋ ASN 205 15.469 -10.473 27.580 1.00 17.26 BLGL ATOM 16.112 -11.622 15.814 -12.907 1501 CA ASN 205 26.964 1.00 17.80 BLGL 1.00 18.45 ATOM 1502 CB ASN 205 27.728 BLGL 16.601 -13.000 ATOM 1503 205 29.001 1.00 18.12 BLGL CG ASN 16.070 -12.811 30.094 1.00 20.78 BLGL ATOM 1504 OD1 ASN 205 17.890 -13.266 15.701 -11.784 1.00 18.03 ATOM 1505 ND2 ASN 205 28.868 BLGL 1.00 17.89 BLGL MOTA 1506 C ASN 205 25.520 ATOM 1507 0 ASN 205 15.129 -12.800 25.135 1.00 18.21 BLGL PRO 206 15.988 -10.771 1.00 18.39 BLGL ATOM 1508 N 24.697 MOTA 1509 CD PRO 206 16.580 -9.480 25,080 1.00 15.66 BLGL 15.657 -10.778 1.00 19.70 BLGL MOTA 1510 CA PRO 206 23.273 MOTA 1511 CB PRO 206 15.903 -9.334 22.867 1.00 19.33 BLGL ATOM 1512 PRO 206 17..029 -8.939 23.756 1.00 16.74 BLGL ĊG ATOM 16.500 -11.748 1513 PRO 206 22.459 1.00 21.36 BLGL C MOTA 1514 PRO 206 16.158 -12.055 21.318 1.00 22.70 BLGL 0 17.601 -12.224 ATOM 1515 N GLU 207 23.034 1.00 23.27 BLGL 1516 22.324 BLGL ATOM GLU 207 18.478 -13.154 1.00 25.47 CA MOTA GLU 207 19.871 -13.210 22.959 1.00 26.18 1517 CB

Fig. 4 cont.

						1 10/			
ATOM	1518	CG	GLU	207		20.021 -12.502	24.288	1.00 30.25	BLGL
ATOM	1519	CD	GLU	207		19.242 -13.139	25.413	1.00 29.52	BLGL
						19.387 -14.353	25.643	1.00 33.25	BLGL
ATOM	1520	OE1		207				1.00 29.56	BLGL
ATOM	1521	QE2	GLU	207		18.495 -12.413	26.081		
MOTA	1522	С	GLU	207.		17.924 -14.561	22.258	1.00 26.20	BLGL
ATOM ·	1523	ō	GLU	207		18.354 -15.357	21.426	1.00 29.50	BLGL
					•	16.982 -14.873	23.139	1.00 25.50	BLGL
MOTA	1524	N	THR	208					BLGL
ATOM	1525	CA	THR	208		16.384 -16.196	23.151	1.00 25.38	
MOTA	1526	CB	THR	208		15.419 -16.349	24.314	1.00 25.02	BLGL
			THR	208		16.108 -16.063	25.532	1.00 24.40	BLGL
ATOM	1527						24.361	1.00 24.75	BLGL
MOTA	1528		THR	208		14.871 -17.765			
ATOM	1529	C ·	THR	208		15.628 -16.435	21.853	1.00 24.66	BLGL
ATOM	1530	0	THR	208		14.689 -15.711	21.531	1.00 23.66	BLGL
	1531	Ν.	SER	209		16.047 -17.455	21.114	1.00 24.67	BLGL
MOTA								1.00 25.56	BLGL
ATOM	1532	CA	SER	209		15.424 -17.791	19.842		
MOTA	1533	CB	SER	209		15.971 -19.120	19.334	1.00 23.59	BLGL
ATOM	1534	OG	SER	209		15.290 -19.524	18.166	1.00 26.21	BLGL
				209		13.896 -17.862	19.885	1.00 26.32	BLGL
ATOM	1535	С	SER					1.00 23.52	BLGL
ATOM	1536	0	SER	209		13.321 -18.668	20.632		•
ATOM	1537	N	GLY	210		13.257 -17.004	19.083	1.00 26.00	BLGL
ATOM	1538	CA	GLY	210	•	11.803 -16.966	18.977	1.00 25.41	BLGL
				210		10.990 -16.593	20.204	1.00 26.60	BLGL
MOTA	1539	С	GLY					1.00 26.52	BLGL
ATOM	1540.	0	GLY	210		9.768 -16.755	20.215		
ATOM.	1541	N	ARG	211		11.659 -16.080	21.231	1.00 27.83	BLGL
ATOM .	1542	CA	ARG	211		11.004 -15.692	22.478.	1.00 25.31	BLGL
				211		12.046 -15.244	23.496	1.00 26.05	BLGL
MOTA	1543	CB	ARG		•			1.00 26.98	BLGL
ATOM	1544	CG	ARG	211		11.487 -15.024	24.881		
ATOM	1545	CD	ARG	211		12.479 -14.289	25.747	1.00 28.49	BLGL
ATOM	1546	NE	ARG	211		12.362 -14.719	27.125	1.00 32.45	BLGL
						13.043 -15.727	27.655	1.00 34.26	BLGL .
MOTA	1547	CZ	ARG	211				1.00 33.07	BLGL
ATOM	1548	NH1	ARG	211		13.903 -16.408	26.920		
ATOM	1549	NH2	ARG	211		12.850 -16.067	28.924	1.00 40.91	BLGL
MOTA	1550	С	ARG	211		9.977 -14.580	22.294	1.00 24.24	BLGL
		ŏ	ARG	211		8.806 -14.744	22.634	1.00 24.47	BLGL
ATOM	1551						21.768	1.00 22.57	BLGL
ATOM	1552	N	TYR	212		10.413 -13.440			
ATOM	1553	CA	TYR	212		9.499 -12.323	21.558	1.00 20.27	BLGL
ATOM	1554	CB	TYR	212		10.262 -11.080	21.093	1.00 18.26	$\mathtt{BLGL}$
MOTA	1555	CG	TYR	212		11.063 -10.409	22.188	1.00 20.40	BLGL
							21.972	1.00 19.09	BLGL
MOTA	1556		TYR	212					
MOTA	1557	CE1	TYR	212		12.387 -8.538	22.982	1.00 16.98	BLGL
ATOM	1558	CD2	TYR	212		11.204 -11.001	23.445	1.00 17.87	BLGL
ATOM	1559	•	TYR	212	•	11.919 -10.377	24.457	1.00 15.68	BLGL
							24.225	1.00 16.21	BLGL
ATOM	1560	CZ	TYR	212					
MOTA	1561	OH	TYR	212		13.200 -8.514	25.235	1.00 15.74	BLGL
MOTA	1562	Ç	TYR	212		8.398 -12.670	20.559	1.00 20.87	BLGL
ATOM	1563	Ó	TYR	212		7.259 -12.237	20.712	1.00 20.22	BLGL
						8.734 -13.449	19.537	1.00 19.68	BLGL
MOTA	1564	N	ALA	213					BLGL
MOTA	1565	CA	ALA	213		7.742 -13.847	18.547	1.00 19.79	
ATOM	1566	CB	ALA	213		8.399 -14.687	17.454	1.00 17.89	BLGL
ATOM	1567	C	ALA	213		6.629 -14.642	19.231	1.00 19.99	BLGL
				213		5.451 -14.479	18.911	1.00 19.71	BLGL
MOTA	1568	O	ALA						BLGL
MOTA	1569	N	TRP	214		7.009 -15.496		1.00 20.09	
MOTA	1570	CA	TRP	214		6.039 -16.309	20.900	1.00 21.30	BLGL
ATOM	1571	CB	TRP	214		6.753 -17.375	21.732	1.00 22.71	BLGL
						5.815 -18.281	22.468	1.00 24.60	BLGL
MOTA	1572	CG	TRP	214					
MOTA	1573	CD2	TRP	214		5.308 -18.094	23.795	1.00 24.97	BLGL
MOTA	1574	CE	TRP	214		4.449 -19.183	24.074	1.00 24.59	BLGL
ATOM	1575		TRP	214		5.496 -17.112	24.775	1.00 25.69	BLGL
						5.256 -19.440		1.00 24.97	BLGL
MOTA	1576		TRP	214					
ATOM	1577		L TRP			4.436 -19.989		1.00 25.84	BLGL
ATOM	1578	CZ	TRP	214		3.780 -19.319	25.294	1.00 22.78	BLGL
ATOM	1579		TRP			4.829 -17.248	25.991	1.00 27.53	BLGL
						3.981 -18.345		1.00 24.84	BLGL
MOTA	1580		TRP	214			_		BLGL
MOTA	1581	C	TRP			5.167 -15.453			
MOTA	1582	0	TRP	214		3.948 -15.630	21.857		BLGL
ATOM	1583	И	ILE			5.793 -14.531			BLGL
001									

Fig. 4 cont.

					150/174	
ATOM	1584	CA	ILE	215	5.067 -13.654 23.469 1.00 19.18	BLGL
ATOM	1585	СВ	ILE	215	6.038 -12.771 24.300 1.00 19.85	BLGL
ATOM	1586	CG2		215	5.257 -11.811 25.198 1.00 15.32 6 930 -13.651 25.170 1.00 18.25	BLGL BLGL
MOTA	1587	CG1		215	6.930 -13.651 25.170 1.00 18.25 7,930 -12.876 25.975 1.00 15.25	BLGL
MOTA	1588	CD1		215 215	4.104 -12.740 22.725 1.00 19.79	BLGL
ATOM	1589 1590	С 0	ILE ILE	215	2.964 -12.550 23.146 1.00 18.73	BLGL
atom Atom	1591	N	ALA	216	4.565 -12.163 21.621 1.00 19.35	BLGL
ATOM .	1592	CA	ALA	216	3.723 -11.275 20.840 1.00 18.57	BLGL
ATOM	1593	СВ	ALA	216	4.492 -10.751 19.650 1.00 18.16	BLGL
MOTA	1594	C	ALA	216	2.472 -12.020 20.378 1.00 20.55	BLGL
MOTA	1595	Ö	ALA	216	1.359 -11.501 20.466 1.00 16.58 2.669 -13.242 19.890 1.00 22.90	BLGL BLGL
MOTA	1596	N	GLU	217 217	2.669 -13.242 19.890 1.00 22.90 1.569 -14.077 19.419 1.00 24.77	BLGL
MOTA	1597 1598	CA CB	GLU GLU	217	2.122 -15.338 18.747 1.00 28.27	BLGL
ATOM ATOM	1599	CG	GLU	. 217	1.063 -16.371 18.379 1.00 33.34	BLGL
ATOM	1600	CD	GLU	217	-0.002 -15.823 17.449 1.00 35.08	BLGL
ATOM	1601	OE1	GLU	217	-1.049 -16.485 17.288 1.00 39.18	BLGL
MOTA	1.602	OE2	GLU	217	0.208 -14.737 16.875 1.00 35.59	BLGL
ATOM	1603	C	GLU	217	0.623 -14.468 20.560 1.00 24.16	BLGL BLGL
ATOM	1604	0	GLU	217	-0.596 -14.464 20.395 1.00 22.67 1.195 -14.805 21.713 1.00 24.08	BLGL
ATOM	1605	N CA	THR THR	218 218	0.412 -15.191 .22.878 1.00 23.79	BLGL
MOTA MOTA	1606 1607	CB	THR	218	1.334 -15.684 24.027 1.00 25.12	. BLGL
ATOM	1608		THR	218	1.985 -16.896 23.630 1.00 26.14	BLGL
ATOM	1609		THR	218	0.537 -15.942 25.298 1.00 23.98	BLGL :
MOTA	1610	С	THR	218	-0.429 -14.014 23.362 1.00 22.94	BLGL
MOTA	1611	0	THR	218	-1.600 -14.179 23.692 1.00 24.35	BLGL BLGL
MOTA	1612	N	LEU	219	0.160 -12.825 23.401 1.00 21.92 -0.578 -11.644 23.846 1.00 23.28	BLGL
MOTA	1613	CA	LEU	219	-0.578 -11.644 23.846 1.00 23.28 0.333 -10.410 23.863 1.00 21.92	BLGL
MOTA ATOM	1614 1615	CB CG	LEU LEU	219 219	1.462 -10.359 24.893 1.00 18.90	BLGL
ATOM	1616		LEU	219	2.386 -9.209 24.570 1.00 14.80	BLGL
ATOM	1617		LEU	219	0.879 -10.220 26.289 1.00 16.33	BLGL
ATOM	1618	С	LEU	219	-1.753 -11.394 22.903 1.00 24.55	BLGL
ATOM	1619	0	LEU	219	-2.850 -11.031 23.322 1.00 25.23	BLGL
ATOM	1620	N	HIS	220	-1.512 -11.603 21.619 1.00 25.34 -2.539 -11.401 20.622 1.00 25.88	BLGL BLGL
MOTA	1621	CA	HIS	220 220	-2.539 -11.401 20.622 1.00 25.88 -1.904 -11.450 19.236 1.00 27.15	BLGL
ATOM ATOM	1622 1623	CB CG	HIS HIS	220	-2.888 -11.366 18.116 1.00 31.81	BLGL
MOTA	1624		HIS	220	-3.485 -10.300 17.529 1.00 31.02	BLGL
MOTA	1625		HIS	220	-3.388 -12.486 17.483 1.00 33.38	BLGL
MOTA	1626	CE1	HIS	220	-4.250 -12.111 16.554 1.00 33.29	BLGL
MOTA	1627		HIS	220	-4.326 -10.791 16.562 1.00 32.86	BLGL
MOTA	1628	C	HIS	220	-3.665 -12.423 20.743 1.00 26.70 -4.839 -12.076 20.617 1.00 25.81	BLGL
MOTA	1629	0	HIS	220 221	-4.839 -12.076 20.617 1.00 25.81 -3.312 -13.679 20.993 1.00 28.18	BLGL
ATOM	1630 1631	N CA	ARG ARG	221	-4.314 -14.730 21.133 1.00 30.04	BLGL
MOTA MOTA	1632	CB	ARG	221	-3.648 -16.090 21.361 1.00 33.95	BLGL
ATOM	1633	CG	ARG	221	-3.038 -16.680 20.095 1.00 40.22	BLGL
ATOM	1634	CD	ARG	221	-2.052 -17.802 20.368 1.00 47.28	BLGL
ATOM	1635	NE	ARG	221	-2.419 -19.012 19.696 1.00 52.72	BLGL
MOTA	1636	CZ	ARG	221	-1.881 -19.711 18.699 1.00 54.00 -2.572 -20.786 18.387 1.00 56.27	BLGL BLGL
MOTA	1637		ARG	221	-2.572 -20.786 18.387 1.00 56.27 -0.762 -19.439 18.032 1.00 52.22	BLGL
ATOM	1638		ARG ARG	221 221	-5.263 -14.440 22.276 1.00 29.71	BLGL
ATOM ATOM	1639 1640	С 0	ARG	221	-6.441 -14.790 22.204 1.00 30.75	BLGL
ATOM	1641	N	HIS	222	-4.757 -13.803 23.331 1.00 27.89	BLGL
ATOM	1642	CA	HIS	222	-5.599 -13.482 24.477 1.00 27.09	BLGL
ATOM	1643	СВ	HIS	222	-4.844 -13.728 25.782 1.00 26.93	BLGL
ATOM	1644	CG	HIS	222	-4.530 -15.168 26.023 1.00 28.56	BLGL
ATOM	1645		HIS	222	-5.196 -16.121 26.716 1.00 30.01	BLGL BLGL
MOTA	1646		L HIS		-3.441 -15.797 25.459 1.00 31.08 -3.448 -17.076 25.792 1.00 30.75	BLGL
ATOM	1647		L HIS 2 HIS		-3.448 -17.076 25.792 1.00 30.75 -4.504 -17.298 26.554 1.00 33.11	BLGL
ATOM ATOM	1648 1649	C	HIS		-6.159 -12.064 24.456 1.00 26.57	BLGL
222 011	-0.2	_				

Fig. 4 cont.

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MOTA

MOTA

MOTA

ATOM

CG2 VAL

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CA

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CG

CD1

CE1

CE2

CZ

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CD2 PHE

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VAL

PHE

ALA

ALA

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### 151/174 25.469 BLGL -6.646 -11.564 1.00 25.69 1650 HIS 222 0 MOTA 1.00 25.18 BLGL -6.084 -11.418 23.300 MOTA 1651 N HIS 223 1.00 26.33 BLGL 23.151 -6.627 -10.082 HIS 223 1652 CA MOTA BLGL 1.00 30.76 -8.147 -10.149 23.214 HIS 223 MOTA 1653 CB 22.309 1.00 38.88 BLGL -8.739 - 11.1821654 HIS 223 ATOM CG 1.00 41.07 BLGL 22.570 -9.524 -12.253 CD2 HIS 223 MOTA 1655 1.00 43,14 BLGL 20.945 -8.531 -11.182 223 1656 ND1 HIS MOTA BLGL -9.161 -12.210 20.405 1.00 43.27 1657 CE1 HIS 223 MOTA BLGL 21.370 1.00 45.48 -9.771 -12.876 NE2 HIS 223 MOTA 1658 BLGL -6.149-9.081 24.186 1.00 26.02 1659 HIS 223 ATOM С BLGL 24.750 1.00 27.73 -6.961 -8.345 1660 ۵ HIS 223 MOTA BLGL 1.00 22.81 24.446 -4.846 -9.044 224 MOTA 1661 N VAL 25.413 1.00 18.14 BLGL -B.096 224 -4.3161662 VAL CA MOTA BLGL 1.00 16.94 -8.499 25.895 -2.912ATOM 1663 CB VAL 224 26.758 1.00 12.94 BLGL -7.399 224 -2.3121664 CG1 VAL MOTA 1.00 15.42 BLGL -9.783 26.676 -2.998 224 MOTA 1665 CG2 VAL 24.734 1.00 17.57 BLGL -6.742 1666 С VAL 224 -4.241MOTA BLGL 1.00 16.83 -6.610 23.646 -3.683 MOTA 1667 0 VAL 224 BLGL -5.738 25.386 1.00 16.35 225 -4.808 1668 N ASP MOTA BLGL 1.00 17.47 -4.393 24.849 -4.820225 ATOM 1669 CA ASP 1.00 17.33 BLGL 25.254 -3.707 1.670 225 -6.123CB ASP MOTA BLGL -2.260 24.843 1.00 19.19 225 -6.172 CG 1671 ASP ATOM 1.00 21.14 BLGL ~1.945 23.717 MOTA 1672 001 ASP 225 -5.722 1.00 19.74. BLGL -6.672 -1.44425.643 225 1673 OD2 ASP ATOM BLGL -3.626 -3.562 25,306 1.00 18.47 ATOM 1674 С ASP 225 BLGL 1.00 19.94 26.433 -3.609-3.073 1675 O ASP 225 ATOM BLGL 24.440 1.00 17.31 -2.626 -3.415226 MOTA 1676 N TYR BLGL -2.610 1.00 19.05 24.762 1677 CA TYR 226 -1.441MOTA BLGL -3.483 25.359 1.00 17.31 -0.315 226 MOTA 1678 CB TYR BLGL 1.00 17.91 -4.417 24.386 MOTA 1679 CG TYR 226 0.380 BLGL -0.315 -5.469 23.780 1.00 17.20 CD1 TYR 226 MOTA 1680 22.891 1.00 14.85 BLGL -6.338 0.317 ATOM 1681 CE1 TYR 226 1.00 15.96 BLGL 226 1.737 -4.253 24.076 1682 CD2 TYR MOTA 1.00 15.01 BLGL -5.117 23.184 2.380 TYR 226 ATOM 1683 CE2 BLGL 1.00 16.47 226 1.661 -6.156 22.598 CZTYR MOTA 1684 2.279 -7.019 21.725 1.00 13.64 BLGL TYR 226 ATOM 1685 OH 1.00 17.95 BLGL -0.944 -1.877 23.513 1686 TYR 226 MOTA C BLGL -1.285 -2.251 22.398 1.00 17.24 MOTA 1687 О TYR 226 1.00 18.09 1.00 20.63 BLGL 23.697 -0.836 227 -0.141 MOTA 1688 N ASP BLGL 227 0.361 -0.075 22,557 ASP ATOM 1689 CA 1.00 23.61 BLGL 22.760 1.424 227 0.126 MOTA 1690 CB ASP BLGL 1.736 23.282 1,00 24.31 227 -1.247MOTA 1691 CG ASP 22.597 1.00 26.42 BLGL -2.242 1.427 227 1692 OD1 ASP MOTA BLGL 1.00 29.59 2.298 24.388 227 -1.327ATOM 1693 OD2 ASP BLGL -0.263 22.289 1.00 21.20 227 1.846 MOTA 1694 С ASP BLGL 1.00 21.63 227 2.283 -0.24121.141 ASP MOTA 1695 0 1.00 21.33 BLGL 2.626 -0.432 23.350 228 MOTA 1696 N VAL 1.00 18.22 BLGL 4.069 -0.571 23.205 228 VAL ATOM 1697 CA 1.00 16.56 BLGL 4.822 0.572 23.961 1698 VAL 228 MOTA CB 1.00 16.51 BLGL 23.669 6.307 0.511 CG1 VAL 228 MOTA 1699

Fig. 4 cont.

1.921

-1.892

-2,338

-2.510

-3.747

-4.694

-6.038

-6.193

-7.141

-7.424

-8.376

-8.516

-3.278

-2.965

-3.205

-2,740

4.268

4.631

4.338

5.444

6.115

6.177

6.773

8.148

5.957

8.698

6.502

7.873

7.517

8.336

7.781

9.076

23.569

23.700

24.811

22.858

23.213

22.007

22.323

22.458

22.537

22.805

22.885

23.020

23.608

22.747

24.909

25.392

1.00 16.96

1.00 16.80

1.00 16.77

1.00 15.66

1.00 16.03

1.00 15.71

1.00 18.72

1.00 20.15

1.00 19.69

1.00 20.33

1.00 19.99

1.00 20.18

1.00 15.51

1.00 16.80

1.00 14.48

1.00 16.32

BLGL

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MOTA

1781

NE1 TRP

### 152/174 BLGL -1.878 26.632 1.00 15.48 230 8.892 ATOM 1716 CB ALA BLGL 25.691 1.00 17.75 -3.878 10.040 1717 ALA 230 ATOM C 1.00 19.06 BLGL 26.019 ALA 230 9.624 -4.990 1718 ATOM 0 BLGL 1.00 15.44 25.580 -3.588SER 231 11.334 ATOM 1719 N 1.00 15.19 BLGL -4.583 25.829 231 12.363 SER MOTA 1720 CA 1.00 12.54 BLGL 24.498 231 12.863 -5,165 ATOM 1721 CB SER BLGL 1.00 9.34 -6.035 24.696 13.966 231 ATOM 1722 OG SER BLGL 26,601 1.00 16.12 -4.024 231 13.554 1723 С SER ATOM BLGL 1.00 17.19 13.915 -2.852 26.463 231 SER MOTA 1724 0 BLGL 27.434 1.00 14.04 MOTA 1725 N SER 232 14.152 -4.865 BLGL -4.463 28.159 1.00 15.04 15.341 232 ATOM 1726 CA SER 1.00 14.50 BLGL 29.447 -5.272 1727 CB SER 232 15.505 ATOM -4.727 30.499 1.00 17.36 BLGL 14.733 232 ATOM 1728 OG SER 1.00 15.02 BLGL 27.216 1729 SER 232 16.485 -4.810C ATOM 16.354 -5.696 26.374 1.00 14.13 BLGL 1730 0 SER 232 ATOM 1.00 14.36 BLGL 27.326 1731 N TYR 233 17.591 -4.094ATOM 18.738 -4.410 26.506 1.00 16.28 BLGL ATOM 1732 CA TYR 233 1,00 15.72 BLGL 18.721 -3.697 25.152 CB TYR 233 ATOM 1733 19.901 -4.146 24.318 1.00 18.38 BLGL 1734 TYR 233 ATOM CG 1.00 17.95 BLGL 19.935 -5.428 23.762 1735 CDI TYR 233 ATOM 1.00 17.74 BLGL 21.072 -5.905 23.102 1736 TYR 233 ATOM CE1 1.00 19.16 BLGL 21.038 -3.342 24.185 233 ATOM 1737 CD2 TYR 1.00 18.72 BLGL -3.809 23.528 22.181 MOTA 1738 CE₂ TYR 233 1.00 20.19 BLGL -5.090 22.991 233 22.188 1739 CZ TYR ATOM BLGL 23.305 ÷5.552 22.339 1.00 21.28 1740 . 233 ATOM OH TYR BLGL 20.051 -4.09627.204 1.00 18.26 1741 TYR 233 ATOM C BLGL 27.282 1.00 19.11 20.488 -2.941TYR 233 ATOM 1742 0 1.00 18.61 BLGL -5.148 27.715 234 20.672 MOTA 1743 N TYR BLGL 1.00 20.22 1744 234 21.951 -5.047 28.382 ATOM CA TYR 1.00 18.03 BLGL -5.594 29.794 234 21.838 1745 CB MOTA TYR 30.678 1.00 19.42 BLGL -4.689 TYR 234 21.020 ATOM 1746 CG BLGL -3.47331.130 1.00 17.03 TYR 234 21.536 1747 CD1 ATOM BLGL -2.628 31.935 1.00 15.84 20.778 1748 TYR 234 ATOM CE1 -5.035 31.051 1.00 20.59 BLGL 234 19.718 CD2 TYR 1749 ATOM BLGL 1.00 18.88 -4.194 31.854 ATOM 1750 CE2 TYR 234 18.950 BLGL -2.995 32.294 1.00 17.70 19,489 CZ234 ATOM 1751 TYR BLGL 1.00 17.67 -2.180 33.108 18.745 MOTA 1752 OH TYR 234 BLGL 234 22.896 -5.875 27.538 1.00 20.87 TYR 1753 С ATOM -7.104 1.00 23.14 BLGL 27.570 MOTA 1754 O TYR 234 22.858 BLGL 23.749 -5.201 26.756 1.00 21.55 235 1755 ATOM N PRO 26.857 1.00 21.91 BLGL 23.983 -3.751 1756 235 ATOM CD PRO -5.825 BLGL 24.728 25.864 1.00 22.81 1757 PRO 235 ATOM ĊA 1.00 22.48 BLGL -4.639 25.367 PRO 235 25.551 MOTA 1758 CB 1.00 21.97 BLGL 25.422 -3.640 26,471 1759 PRO 235 ATOM CG 1.00 23.83 BLGL -6.912 26.508 ATOM 1760 С PRO 235 25.575 -7.762 -6.894 BLGL 1.00 26.44 235 26.118 25.812 1761 PRO MOTA 0 1.00 24.38 BLGL 27.834 236 25.673 MOTA 1762 N PHE BLGL -7.894 1.00 23.56 PHE 236 26.451 28.556 ATOM 1763 CA 1.00 22.41 BLGL 30.069 236 26.439 -7.613 ATOM 1764 CB PHE 26.751 1.00 20.97 BLGL -6.190 30.432 1765 PHE 236 ATOM CG 1.00 22.30 BLGL 236 25.769 -5.363 30.960 1766 CD1 PHE ATOM 1.00 21.90 BLGL -5.666 30.224 28.018 **ATOM** 1767 CD2 PHE 236 BLGL 1.00 20.76 1768 26.043 -4.031 31.274 CE1 PHE 236 ATOM BLGL 28.304 -4.335 30.534 1.00 22.34 ATOM 1769 CE2 PHE 236 1.00 22.41 BLGL -3.51831.060 PHE 236 27.310 ATOM 1770 CZ BLGL 1.00 24.55 -9.297 28.322 ATOM 1771 С PHE 236 25.901 26.664 -10.252 28.209 1.00 26.43 BLGL 1772 236 0 PHE ATOM BLGL 24.581 -9.425 1.00 25.33 28.226 ATOM 1773 N TRP 237 BLGL 23.971 -10.745 28.067 1.00 26.98 1774 TRP 237 CA ATOM 1.00 27.82 BLGL 23.270 -11.144 29.367 MOTA 1775 CB TRP 237 30.606 1.00 30.90 BLGL 1776 CG 237 23,960 -10,698 MOTA TRP 1.00 31.06 BLGL ~9.632 31.466 ATOM 1777 CDZ TRP 237 23.562 BLGL 24.489 -9.585 32.535 1.00 31.99 237 1778 CE2 TRP MOTA 1.00 32.34 BLGL 237 22.511 -8.711 31.443 MOTA 1779 CE3 TRP 1.00 33.44 BLGL 237 25.084 -11.238 31.162 CD1 TRP ATOM 1780 1.00 32.26 32.324 237 25.408 -10.577

Fig. 4 cont.

						15	3/1/4			
MOTA	1782	CZ2	TRP	237			-8.652	33.570	1.00 32.74	BLGL
ATOM	1783	CZ3		237			-7.780	32.477	1.00 34.34	BLGL
MOTA	1784	CH2		237 .		23.357	-7.761	33.526	1.00 33.93	BLGL
MOTA	1785	_	TRP	237		22.938 ~	10.894	26.960	1.00 26.05	BLGL BLGL
ATOM	1786		TRP	237		22.632 -		26.543	1.00 25.25 1.00 24.70	BLGL
MOTA	1787		HIS	238	•		-9.778	26.487	1.00 20.96	BLGL
ATOM	1788		HIS	238			-9.824	25.504 25.824	1.00 20.90	BLGL
MOTA	1789		HIS	238			-8.703	27.192	1.00 17.38	BLGL
MOTA	1790		HIS	238		19.772 19.601	-8.821 -9.900	27.192	1.00 16.73	BLGL
MOTA	1791	CD2		238		19.291	-7.743	27.896	1.00 20.29	BLGL
ATOM	1792	ND1		238 238		18.850	-8.151	29,073	1.00 20.03	BLGL
ATOM ATOM	1793 1794	CE1 NE2		238		19.026	-9.456	29.154	1.00 19.52	BLGL
ATOM	1795		HIS	238		21.628	-9.863	24.019	1.00 20.65	BLGL
ATOM	1796		HIS	.238		20.854	-9.354	23.217	1.00 22.38	BLGL
ATOM	1797	N	GLY	239		22.730 -	-10.489	23.643	1.00 19.61	BLGL
ATOM	1798	CA	GLY	239		23.037 -	-10.607	22,234	1.00 19.09	BLGL
ATOM	1799		GLY	239		23.345	-9.338	21.474	1.00 18.09	BLGL
ATOM	1800	0	GLY	239		23.535	-8.271	22.046	1.00 17.84	BLGL
MOTA	1801	N	THR	240		23.369	-9.476	20.158	1.00 17.37	BLGL ·
MOTA	1802	CA	THR	240		23.697	-8.387	19.258	1.00 18.95	BLGL
MOTA	1803	CB	THR	240		24.139	-8.949	17.896	1.00 18.49	BLGL
ATOM	1804	OG1			٠.	-23.028	-9.589	17.262	1.00 18.33	BLGL BLGL
MOTA	1805	CG2		240		25.239	-9.964	18.076	1.00 14.06	BLGL
MOTA	1806	С	THR	240 '		22.610	-7.348	19.003 19.169	1.00 20.98 1.00 19.90	BLGL
MOTA	1807	0	THR	240		21.418	-7.604 -6.165	18,581	1.00 21.55	BLGL
MOTA	1808		LEU	241		· 23.043 22.115	-5.094	18.277	1.00 21.65	BLGL
MOTA	1809	.CA	LEU	241 241		22.115	-3.780	18.086	1.00 20.04	BLGL
MOTA	1810 1811	CB CG	LEU LEU	241		23.464		19.381	1.00 21.24	BLGL
ATOM ATOM	1812		LEU			24.455	-2.105	19.074	1.00 18.53	BLGL
ATOM	1813		LEU	241		22.339	-2.689	20.259	1.00 19.54	BLGL
MOTA	1814	C	LEU	241		21.350	-5.458	17.011	1.00 22.88	BLGL
ATOM	1815	ō	LEU	241		20.213	-5.043	16.827	1.00 23.81	BLGL
ATOM	1816	N	LYS	242		21.971	-6.248	16.143	1.00 23.90	BLGL
ATOM	1817	CA	LYS	242	•	21.322	-6.659	14.902	1.00 25.71	BLGL
ATOM	1818	CB	LYS	242		22.314	-7.426	14.025	1.00 30.56	BLGL
MOTA	1819	CG	LYS	242		21.771		12.670	1.00 36.92	BLGL
MOTA	1820	CD	TA2	242		22.735	-8.821	11.983	1.00 43.60	BLGL BLGL
ATOM	1821	CE	LYS	242		22.175	-9.333	10.664	1.00 48.93 1.00 51.96	BLGL
ATOM	1822	NZ	LYS	242		21.895	-8.217 -7.537	9.709	1.00 24.37	BLGL
ATOM	1823	Ċ	LYS	242		20.108 19.070	-7.444	14.551	1.00 23.45	BLGL
ATOM	1824	0	LYS ASN	242 243	•	20.248	-8.384	16.219	1.00 23.09	BLGL
ATOM	1825 1826	N CA	ASN	243		19.178	-9.279	16.637	1.00 21.13	BLGL
MOTA MOTA	1827	CB	ASN	243			-10.285	17.653	1.00 20.66	BLGL
ATOM	1828	CG	ASN	243			-11.196	18.185	1.00 22.04	BLGL
ATOM	1829		ASN	243		18.181	-12.102	17.495	1.00 21.37	BLGL
ATOM	1830		ASN	243			-10.951	19.415	1.00 21.96	BLGL
ATOM	1831	С	ASN	243		18.041	-8.477	17.264	1.00 21.16	BLGL
ATOM	1832	0	ASN	243		16.861	-8.684	16.957	1.00 18.33	BLGL
ATOM	1833	N	LEU	244		18.408	-7.557		1.00 20.72	BLGL
ATOM	1834	CA	LEU	244		17.429	-6.712			BLGL
ATOM	1835	CB	LEU	244		18.131	-5.667	19.695		BLGL
ATOM	1836		LEU	244		17.188	-4.669			BLGL
ATOM	1837		LEU	244		16.393	-5.385			BLGL BLGL
ATOM	1838		LEU	244		17.995	-3.515			BLGL
ATOM	1839		LEU	244		16.565	~6.000			BLGL
ATOM	1840	0	LEU	244		15.341	-6.054			BLGL
ATOM	1841		THR	245		17.214	-5.332	_		BLGL
ATOM	1842		THE	245		16.505	-4.606 -3.996			BLGL
ATOM	1843		THR	245		17.474 18.318	-3.930			BLGL
ATOM	1844		THR THR			16.697	-3.311			BLGL
ATOM ATOM	1845 1846		THR			15.574	-5.531			BLGL
ATOM	1847		THR			14.410	-5.219			BLGL
	,	-								

Fig. 4 cont.

### 154/174 BLGL -6.678 14.678 1.00 20.39 1848 246 16.109 ATOM N SER BLGL 246 15.361 -7.661 13.927 1.00 19.04 1849 SER MOTA CA 1.00 18.29 BLGL -8.792 13.538 16.303 246 ATOM 1850 CB SER BLGL 246 15.593 -9.911 13.053 1.00 23.84 ATOM 1851 OG SER 14.695 1.00 20.89 BLGL -8.205 246 14.164 ATOM 1852 С SER BLGL 13.034 -8.169 14.214 1.00 22.76 246 ATOM 1853 0 SER -8.703 1.00 21.65 BLGL 15.899 1854 247 14.411 ATOM N VAL BLGL 1.00 21.83 -9.280 16.701 1855 247 13.343 MOTA CA VAL BLGL -9.883 18.005 1.00 20.50 1856 VAL 247 13.923 MOTA CB BLGL 1.00 20.71 VAL 247 14.342 -8.786 18.962 MOTA 1857 CG1 BLGL -10.80018.636 1.00 23.56 12.912 MOTA 1858 CG2 VAL 247 BLGL 17.006 1.00 22.43 12.215 -8.275 1859 247 ATOM С VAL 1.00 22.15 BLGL 11.031 ÷8.631 17.000 MOTA 1860 0 VAL 247 BLGL 1.00 22.41 12.578 -7.020 17.255 LEU 248 MOTA 1861 N 1.00 22.55 BLGL 17.538 11.584 -5.990 MOTA 1862 CA LEU 248 BLGL 12.251 -4.73418.125 1.00 20.88 ATOM 248 1863 CB LEU 1.00 19.44 BLGL 12,778 19.563 248 -4.816 MOTA 1864 CG LEU 1.00 17.12 BLGL 13.426 -3.498 19.954 ATOM LEU 248 1865 CD1 -5.143 20.505 1.00 15.29 BLGL 11.639 MOTA 1866 CD2 LEU 248 BLGL 16.270 1.00 23.02 10.805 -5.617 1867 LEU 248 ATOM C 16.318 1.00 22.01 BLGL 9.597 -5.381 MOTA 1868 0 LEU 248 BLGL 249 11.496 -5.570 15.136 1.00 20.49 MOTA 1869 N THR 13.890 1.00 21.29 BLGL 10.844 -5.220 249 **ATOM** 1870 CA THR 12.722 1.00 22.20 BLGL 249 11.836 -5.197 ATOM 1871 CB THR BLGL 249 12.872 -4.246 12.994 1.00 24.83 OG1 THR ATOM 1872 11.440 1.00 20.47 BLGL -4.808 1873 CG2 THR 249 11.128 ATOM -6.214 13.573 1.00 22.84 BLGL 249 9.739 1874 С THR ATOM 1.00 20.69 BLGL 8.706 -5-842 13.020 MOTA 1875 0 THR 249 9.956 -7.481 13.920 1.00 23.97 BLGL 1876 250 ATOM N SER BLGL -8.509 13.667 1,00 25.77 8.945 MOTA 1877 CA SER 250 BLGL 1878 250 9.451 -9.889 14.076 1.00 27.18 CB SER ATOM 1.00 34.71 BLGL 10.487 -10.310 13.213 250 ATOM 1879 OG SER 1.00 24.53 BLGL 1880 C SER 250 7.686 ~8.196 14.446 ATOM 1.00 24.89 BLGL 250 6.590 -8.207 13,892 ATOM 1881 O SER BLGL 1.00 22.02 -7.919 15.736 MOTA 1882 N JAV 251 7.850 -7.592 -7.246 6.713 16.581 1.00 20.32 BLGL 251 ATOM 1883 CA VAL 1.00 19.00 BLGL 1884 VAL 251 7.156 18.022 ATOM CB BLGL 5.972 -6.733 18.822 1.00 19.03 VAL 251 ATOM 1885 CG1 18.693 1.00 17.23 BLGL -8.475 7.736 1886 VAL 251 ATOM CG2 1.00 20.70 BLGL 1887 С VAL 251 5.968 -6.401 15.984 ATOM 4.741 -6.399 15.912 1.00 20.26 BLGL ATOM 1888 0 VAL 251 1.00 20.84 BLGL 6.717 -5.396 15.546 1889 ALA 252 MOTA N 1.00 21.97 14.965 BLGL 6.123 ~4.198 ATOM 1890 ALA 252 CA BLGL 1.00 21.24 7.203 -3.17514.663 ATOM 1891 CB ALA 252 BLGL 5.330 -4.497 13.701 1.00 22.61 ATOM 1892 С ALA 252 BLGL 1.00 23.36 1893 ALA 252 4.137 -4.219 13,629 ATOM O 5.999 1.00 22.58 BLGL -5.069 12.711 253 ATOM 1894 N ASP 1.00 23.48 BLGL 11.440 253 5.366 -5.386 MOTA 1895 CA ASP 10.472 1.00 23.27 BLGL ASP 253 6.394 -5.968 **ATOM** 1896 CB 1.00 25.67 BLGL 10.019 7.403 -4.946 ATOM 1897 CG ASP 253 8.372 -5.346 9.337 1.00 26.60 BLGL ATOM 1898 OD1 ASP 253 1.00 27.47 BLGL 1899 ASP 253 7.224 -3.74410.344 MOTA OD2 11.556 1.00 24.77 BLGL 4.203 -6.352ATOM ASP 253 1900 C 1.00 25.85 BLGL 3.174 -6.174 10.904 1901 ASP 253 ATOM 0 BLGL -7.371 12.389 1.00 24.09 1902 THR 254 4.359 ATOM N -8.374 1.00 22.38 BLGL 12.537 1903 CA THR 254 3.317 MOTA BLGL 3.892 13.094 1.00 21.12 254 -9.679 1904 THR MOTA CB 1.00 22.06 BLGL MOTA 1905 OG1 THR 254 5.000 -10.096 12.287 BLGL 2.836 -10.765 13.073 1.00 20.31 ATOM CG2 THR 254 1906 1.00 23.11 BLGL -7.977 13.395 MOTA 1907 THR 254 2.123 BLGL 1908 THR 254 0.995 -8.366 13.102 1.00 26.89 0 **ATOM** -7.201 1.00 21.45 BLGL 14.444 ATOM 1909 Ν TYR 255 2.345 BI.GL 1.231 -6.835 15.307 1.00 20.15 MOTA 1910 CA TYR 255 BLGL 1.488 -7.377 16.709 1.00 20.87 255 ATOM 1911 CB TYR

Fig. 4 cont.

-8.876

-9.728

16,701

16,56B

1.00 22.40

1.00 21.45

1.670

0.568

1912

1913

ATOM

ATOM

CG

TYR

CD1 TYR

255

255

BLGL

MOTA

1979

N

### 155/174 0.731 -11.107 1.00 21.01 BLGL 16.494 1914 CE1 TYR 255 MOTA -9.443 16.761 1.00 19.96 BLGL 2.943 255 1915 CD2 TYR MOTA 1.00 20.59 BLGL 3.117 -10.822 16.686 255 1916 TYR ATOM CE₂ BLGL 16.554 1.00 21.17 2.008 -11.647 255 TYR 1917 CZ ATOM 1.00 21.44 BLGL 2.179 -13.009 16.495 191B TYR 255 ATOM OH 15.360 1.00 19.29 BLGL 0.927 -5.357 255 TYR 1919 C ATOM BLGL -4.923 16.104 1.00 19.71 0.056 MOTA 1920 0 TYR 255 14.562 1.00 20.06 BLGL 1.649 -4.585 256 ATOM 1921 N GLY BLGL -3.15514.516 1.00 21.23 1.421 1922 CA GLY 256 ATOM 1.00 21.40 BLGL 256 1.582 -2.45415.847 GLY MOTA 1923 C 1.00 22.35 BLGL -1.593 16.212 0.788 ATOM 1924 O GLY 256 1.00 20.19 BLGL 257 2.619 -2.815 16.5Bl LYS ATOM 1925 N 1.00 21.01 BLGL 2.845 17.861 -2.182 257 1926 CA LYS ATOM 1.00 20.86 BLGL 3.032 -3.24418.949 CB 257 MOTA 1927 LYS 19.122 1.00 18.58 BLGL -4.191 257 1.863 ATOM 1928 CG LY\$ BLGL 1.00 17.81 257 0.615 -3.458 19.566 LYS MOTA 1929 CD 19.765 1.00 16.84 BLGL -4.428 -0.524 1930 CE LYS 257 ATOM BLGL 1.00 19.74 -3.739 20.053 257 -1.801 LYS ATOM . 1931 NZ -1.300 17.792 1.00 20.95 BLGL 257 4.082 1932 С LYS ATOM 1.00 19.83 BLGL -1.47416.918 LYS 257 4.934 MOTA 1933 0 18.699 BLGL 1.00 19.92 -0.333 258 4.161 1934 N LYS ATOM 1.00 21.02 BLGL 0.526 18.771 5.329 LYS 258 ATOM 1935 CA 1.00 24.26 . BLGL 1.785 19.581 1936 CB LYS 258 5.037 MOTA BLGL 3.850 1.00 27.83 2.601 19.139 LYS 258 ATOM 1937 ĊĠ BLGL 3.387 17.887 1.00 33.22 258 4.143 1938 CD LYS · ATOM 1.00 36.49 BLGL 4.652 17.862 258 3.297 MOTA 1939 CE LYS 1.00 38.07 BLGL 18.036 4.362 258 1.845 1940 NZ LYS ATOM 1.00 21.33 BLGL. -0.326 19.559 6.322 MOTA 1941 C LYS 258 20.276 BLGL 1.00 21.62 258 5.923 -1.2481942 0 LYS ATOM BLGL 1.00 18.75 -0.037 19.430 7.607 259 AT:OM 1943 N VAL 20.176 1.00 17.87 BLGL -0.786 259 8.604 MOTA 1944 CA VAL BLGL 19.271 . 1.00 17.66 9.391 -1.762 259 VAL ATOM 1945 CB 1.00 16.47 BLGL 18.686 -2.789 CG1 VAL 259 8.447 ATOM 1946 -0.997 18.171 1.00 16.36 BLGL 10.118 259 CG2 VAL ATOM 1947 BLGL 20.816 1.00 18.60 0.190 MOTA 1948 C VAL 259 9.572 1.00 19.89 BLGL 1.362 20.443 9.628 ATOM 1949 0 VAL 259 BLGL 1.00 18.23 21.794 -0.280 ATOM 1950 MET 260 10.328 N BLGL 11.295 0..583 22.452 1.00 18.93 260 MET MOTA 1951 CA 1.00 17.82 BLGL 23.179 1.741 ATOM 1952 ÇB MET 260 10.594 BLGL 9.861 1.335 24.450 1.00 18.62 260 ATOM 1953 CG MET 25.444 BLGL 1.00 20.82 2.760 9.338 ATOM 1954 SD MET 260 BLGL 1.00 14.70 9.092 1.989 27.061 MET 260 MOTA 1955 CE 1.00 18.97 BLGL 23.461 -0.200 260 12.109 ATOM 1956 С MET 1.00 18.84 · BLGL -1.326 23.827 11.757 260 ATOM 1957 0 MET 23.900 1.00 18.49 BLGL 0.401 195B N VAL 261 13.207 MOTA BLGL 1.00 19.01 24.907 261 14.049 -0.215VAL ATOM 1959 CA -0.063 24.567 1.00 18.88 BLGL 15.545 261 MOTA 1960 CB VAL BLGL -0.549 25.728 1.00 19.31 261 16.399 ATOM 1961 CG1 VAL BLGL 23.326 1.00 17.95 -0.867 1962 15.867 VAL 261 ATOM CG2 26.218 1.00 17.97 BLGL 13.713 0.493 VAL 261 ATOM 1963 C BLGL 1.00 14.60 13.854 1.712 26.343 1964 VAL 261 ATOM 0 BLGL 27.180 1.00 18.80 -0.280 262 13.228 MOTA 1965 N ALA 1.00 21.56 28.473 BLGL 1966 12.846 0.269 ALA 262 CA ATOM BLGL 29.107 1.00 20.01 11.777 -0.617 ATOM 1967 CB ALA 262 BLGL 1.00 21.77 29.412 14.047 0.409 1968 ALA 262 ATOM Ç BLGL 30.262 1.00 22.42 14.079 1.297 ATOM 1969 0 ALA 262 1.00 20.47 BLGL 15.036 -0.464 29.247 1970 GLU 263 N MOTA BLGL 16.214 30.091 1.00 19.18 -0.433ATOM 1971 ÇA GLU 263 1.00 18.99 BLGL 16.099 -1.464 31.211 GLU 263 1972 CB ATOM BLGL 32,358 1.00 21.05 15.178 -1.102 MOTA 1973 ÇG GLU 263 1.00 19.91 BLGL -2.191 33.417 GLU 263 15.151 1974 CD MOTA 1.00 20.67 BLGL 33.642 16.207 -2.8191975 OE1 GLU 263 MOTA BLGL 1.00 22.21 14.087 -2.422 34.029 OE2 GLU 263 ATOM 1976 29.319 BLGL 1.00 19.96 263 17.483 -0.729ATOM 1977 С GLU BLGL -1.587 1.00 20.56 17.497 28.440 263 ATOM 1978 0 GLU 29.661 1.00 17.62 BLGL -0.013THR 264 18.547

Fig. 4 cont.

					15	6/174			
ATOM	1980	CA	THR	264	19.844	-0.219	29.042	1.00 15.98	BLGL
ATOM	1981		THR	264	19.874	0.247	27.573	1.00 16.21	BLGL
ATOM	1982	OG1	THR	264	20.989	-0.366	26.907	1.00 15.60	BLGL
MOTA	1983	CG2		264	20.036	1.771 0.578	27.494 29.820	1.00 13.52 1.00 15.21	BLGL BLGL
ATOM	1984.	C	THR	264	20.872 20.532	1.477	30.579	1.00 13.21	BLGL
MOTA	1985	о И	THR SER	264 265	22.136	0.240	29.621	1.00 15.34	BLGL
ATOM ATOM	1986 1987	CA	SER	265	23.229	0.936	30.280	1.00 16.34	BLGL
ATOM	1988	CB	SER	265	23.113	0.819	31.802	1.00 16.26	BLGL
ATOM	1989	OG	SER	265	23.293	-0.517	32.249	1.00 16.64	BLGL
MOTA	1990	С	SER	265	24.531	0.312	29.826	1.00 17.34	BLGL BLGL
ATOM	1991	0	SER	265	24.543	-0.607 0.836	29.005 30.349	1.00 18.70 1.00 18.17	BLGL '
ATOM	1992	N	TYR TYR	· 266 266	25.629 26.939	0.307	30.039	1.00 17.93	BLGL
ATOM ATOM	1993 1994	CA · CB	TYR	266	27.397	0.699	28.640	1.00 15.84	BLGL
	: 1995	CG	TYR	266 .	28.485	-0.218	28.131	1.00 17.82	·BLGL
MOTA	1996		TYR	266	28.192	-1.527	27.774	1.00 18.54	BLGL
MOTA	1997	CEl	TYR	266	29.186	-2.396	27.329	1.00 19.26	BLGL
ATOM	1998		TYR	266	29.816	0.210	28.035	1.00 20.22 1.00 19.11	BLGL BLGL
ATOM	1999	CE2	TYR	266	30.826 30.499	-0.656 -1.962	27.591 27.238	1.00 19.11	BLGL
MOTA	2000 2001	CZ OH	TYR TYR	266 266	31.472	-2.836	26.784	1.00 18.36	BLGL
ATOM ATOM	2001	C	TYR	266	27.911	0.846	31.064	1.00 18.90	Brèr
ATOM	2003	ō	TYR	266	27.681	1.895	31.665	1.00 18.09	BLGL
MOTA	2004	N	THR	267	28.995	0.105	31.259	1.00 20.38	BLGL
MOTA	2005	CA	THR	267	30.037	0.462	32.210	1.00 21.04	BLGL BLGL
ATOM	2006	CB	THR	267	30.852	-0.773 -1.402	32.580 31.373	1.00 20.00	BLGL
	2007 2008	· OG1 CG2		267 267	31.305 30.017	-1.752	33.366	1.00 19.30	BLGL
ATOM ATOM	2008	C	THR	267	31.000	1.482	31.619	1.00 21.49	BLGL
ATOM	2010	ŏ	THR	267	31.455	1.315	30.488	1.00 24.81	BLGL
MOTA	2011	N	TYR	268	31.320	2.525	32.384	1.00 20.55	BLGL
ATOM	2012	CA	TYR	268	32.268	3.546	31.933	1.00 20.98	BLGL
MOTA	2013	CB	TYR	268	31.724	4.958 5.439	32.205 33.639	1.00 21.01 1.00 19.32	BLGL BLGL
MOTA	2014	CG	TYR TYR	268 268	31.844 33.019	6.027	34.105	1.00 20.87	BLGL
ATOM ATOM	.2015 2016		TYR	268	33.129	6.471	35.426	1.00 20.17	. BLGL
ATOM	2017		TYR	268	30.778	5.302	34.532	1.00 21.37	BLGL
ATOM	2018	CE2	TYR	268	30.873	5.739	35 <b>.853</b>	1.00 19.23	BLGL
ATOM	2019	CZ	TYR	268	32.049	6.322	36.295	1.00 21.74	BLGL BLGL
ATOM	2020	ОН	TYR	268	32.137	6,753 3.364	37.604 32.664	1.00 22.30 1.00 21.83	BLGL
ATOM	2021	C.	TYR TYR	268 268	33.597 34.590	4.013	32.344	1.00 18.94	BLGL
MOTA MOTA	2022 2023	N O	THR	269	33.600	2.479	33.657	1.00 22.82	BLGL
ATOM	2024	CA	THR	269	34.795	2.213	34.451	1.00 23.10	BLGL
ATOM	2025	CB	THR	269	34.970	3.271	35.573	1.00 20.44	BLGL
ATOM	2026		THR	269	36.161	2.989	36.311	1.00 20.91	BLGL BLGL
MOTA	2027		THR	269	33.791	3.250	36.524	1.00 18.84 1.00 23.00	BLGL
ATOM	2028	C	THR	269 269	34.693 33.607	0.834 0.376	35.083 35.403	1.00 25.15	BLGL
MOTA MOTA	2029 2030	О И	THR ALA	270	35.826	0.170	35.259	1.00 24.31	BLGL
ATOM	2030	CA	ALA		35.825	-1.158	35.853	1.00 24.71	BLGL
ATOM	2032	СВ	ALA		37.058	-1.933	35.409	1.00 21.17	BLGL
MOTA	2033	C	ALA		35.810	-1.019	37.361	1.00 25.78	BLGL
MOTA	2034	0	ALA		35.538	-1.970	38.080	1.00 29.18	BLGL BLGL
ATOM	2035	N	GLU		36.083	0.185	37.836 39.263	1.00 27.12	BLGL
ATOM	2036	CA	GLU		36.133 36.914	0.448 1.742		1.00 32.08	BLGL
MOTA MOTA	2037 2038	CB CG	GLU		36.864	2,261		1.00 35.54	BLGL
ATOM	2038	CD	GLU		37.750	3.466	_	1.00 36.58	BLGL
MOTA	2040		L GLU		38.022	4.167		1.00 36.10	BLGL
ATOM	2041		GLU	271	38.160	3.714	42.262	1.00 38.61	BLGL
ATOM	2042	C	GLU		34.783	0.527		1.00 30.16	BLGL BLGL
ATOM	2043	0	GLU		33.776	0.938		1.00 31.60 1.00 30.13	BLGL
ATOM	2044	N	ASP		34.782 33.590	0.125 0.169		1.00 30.13	BLGL
ATOM	2045	CA	SZA	272	33.330				

Fig. 4 cont.

### 157/174 1.00 29.68 BLGL 33.333 -1.190 42.722 ASP 272 2046 CB ATOM BLGL 1.00 29.93 43.968 272 32.488 -1.081 2047 ASP ATOM CG 43.896 BLGL -0.428 1.00 29.02 31.427 2048 OD1 ASP 272 MOTA BLGL 32.884 -1.640 45.014 1.00 30.80 272 OD2 ASP 2049 MOTA BLGL 33.865 1.188 43.178 1.00 31.65 272 2050 ASP C MOTA BLGL 0.946 44,045 1.00 33.92 34.705 2051 0 ASP 272 ATOM 43.157 1.00 31.58 BLGL 33.163 2.318 273 2052 GLY М MOTA 3.340 44.158 1.00 32.18 BLGL 33.420 2053 CA GLY 273 MOTA 1.00 31.14 BLGL 32.476 3.304 45.333 2054 С GLY 273 ATOM BLGL 4.250 46.116 1.00 32.09 32.407 ATOM 2055 0 GLY 273 45.472 1.00 30.99 BLGL 274 31.786 2.184 ASP 2056 ATOM N 1.00 30.40 BLGL 274 30.790 2.002 . 46.511 MOTA 2057 CA AS2 1.00 31.29 BLGL 29.550 1.377 45.871 ASP 274 ATOM 2058 CB 1.00 32.35 BLGL 28.304 1.620 46.659 274 MOTA 2059 ÇG ASP 1.00 34.84 BLGL ASP 274 27.319 0.902 46.433 2060 OD1 MOTA 47.495 1.00 38.43 BLGL 28.299 2.539 274 ATOM 2061 OD2 ASP 1.00 30.15 BLGL 47.649 ASP 274 31.264 1.104 2062 С MOTA 31.075 48.827 1.00 28.39 BLGL 1.408 274 2063 0 ASP MOTA 1.00 28.33 BLGL 47.283 2064 GLY 275 31.867 -0.017 ATOM N -0.956 48.283 1.00 29.05 BLGL 32.311 275 2065 CA GLY **ATOM** 1.00 28.72 BLGL 31.486 -2.210 48.099 2066 C GLY 275 MOTA -3.29848.519 1.00 31.31 BLGL 31.881 2067 Q GLY 275 ATOM 1.00 26.86 BLGL 47.472 276 30.325 -2.046 2068 HIS ATOM N 29.431 -3.164 47.191 1.00 24.43 BLGL 276 2069 CA HIS MOTA 1.00 23.89 BLGL 47.336 27.974 -2.726MOTA 2070 CB HIS 276 BLGL 1.00 26.16 2.76 26.986 -3.842 47.172 ATOM 2071 CG HIS BLGL 46.078 1.00 24.85 276 26.329 -4.297 MOTA 2072 CD2 HIS 1.00 26.36 BLGL 276 26.595 -4.652 48.217 2073 ND1 HIS MOTA BLGL 47.776 1,00 24.78 25.741 -5.557 CE1 HIS 276 ATOM 2074 46.481 1.00 25.01 BLGL -5.363 25.562 2075 NE2 HIS 276 MOTA 29.691 1.00 24.24 BLGL 45,748 2076 HIS 276 -3.597 С MOTA 1.00 23.66 BLGL 29.512 -2.808 44.822 276 MOTA 2077 0 HIS 1.00 23.41 BLGL 277 30.108 -4.844 45.562 2078 GLY N MOTA 1.00 23.85 BLGL -5.343 44.225 2079 CA GLY 277 30.397 MOTA BLGL 1.00 24.88 277 29.405 -4.987 43.130 GLY MOTA 2080 С 1.00 25.03 BLGL -5.064 43.320 28.185 MOTA 2081 0 GLY277 1.00 24.25 BLGL 29.935 -4.616 41.966 ASN 278 MOTA 2082 N 1.00 22.79 BLGL -4.238 40.822 29.114 **ATOM** 2083 CA ASN 278 BLGL 40.027 1.00 21.96 278 29.827 -3.1502084 CB ASN MOTA -1.844 1.00 23.90 BLGL 278 29.928 40.797 ATOM 2085 CĢ ASN 1.00 26.25 BLGL 278 30.661 -0.93440.410 2086 ND2 ASN MOTA 1.00 21.34 BLGL 29.177 -1.74241.889 278 ATOM 2087 OD1 ASN BLGL -5.407. 39.910 1.00 23.33 2088 ASN 278 28.748 ATOM C -6.443 1.00 22.97 BLGL 278 29.408 39.898 ATOM 2089 0 ASN 1.00 23,75 BLGL -5.226 ATOM 2090 N THR 279 27.675 39.152 27.188 -6.247 38.241 1.00 24.46 BLGL 279 ATOM 2091 CA THR 1.00 25.31 BLGL -5.857 37.666 MOTA 2092 CB THR 279 25.821 BLGL 24.874 -5.729 38.728 1.00 27.04 279 ATOM 2093 OG1 THR 1.00 28.22 BLGL -6.91036.701 279 25.331 ATOM 2094 CG2 THR BLGL -6.482 37,078 1.00 24.01 28.137 ATOM 2095 THR 279 C 1.00 24.35 BLGL 36.659 279 28.356 -7.6132096 ٥ THR ATOM 28.687 -5.401 36.547 1.00 24.16 BLGL 280 2097 ALA ATOM N 1.00 24.11 BLGL ALA 280 29.599 -5.495 35.422 ATOM 2098 CA 1.00 21.63 BLGL 28.857 -5.182 34.137 2099 CB ALA 280 ATOM BLGL 1.00 25.17 30.749 -4.522 35.616 2100 280 ATOM C ALA 30.638 1.00 26.21 BLGL -3.565 36.379 ATOM 2101 ALA 280 1.00 25.93 BLGL -4.766 31.881 34.942 2102 PRO 281 MOTA N 1.00 26.64 BLGL -3.790 34.829 32.977 ATOM 2103 CD PRO 281 1.00 27.75 BLGL PRO 281 32.106 -5.896 34.037 CA MOTA 2104 BLGL 33.084 1.00 27.25 33.155 -5.353 MOTA 2105 CB PRO 281 1.00 28.42 BLGL 2106 -4.545 33.998 281 34.001 CG PRO ATOM -7.142 BLGL 32.590 34.773 1.00 29.21 PRO 281 ATOM 2107 Ċ BLGL -7.071 35.902 1.00 31.08 33.055 0 PRO 281 ATOM 2108 1.00 31.67 BLGL 34.123 282 32.468 -8.287 ATOM 2109 N LYS

Fig. 4 cont.

31.788 -10.169

-9.546

32.902

282

282

CA

2110

2111

MOTA

ATOM

LYS

LYS

34.705

35.537

1.00 35.33

1.00 34.90

BLGL

2168

2169

2170

2171

2172

2173

2174

2175

2176

2177

C

0

N

CD

CA

CB

CG

С

0

N

ATOM

ATOM

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33.818

33.698

34.815

35.116

35.783

36.796

35.977

35.098

34.140

35.582

### 158/174 31.527 -9.495 36.861 1.00 37.13 BLGL 282 LYS MOTA 2112 CG 1.00 38.88 BLGL 37.636 282 30.496 -10.301 LYS ATOM 2113 CD BLGL 30.386 -9.846 39.077 1.00 40.27 ATOM 2114 ĊE LYS 282 1.00 42.22 BLGL 29.540 -10.796 39.851 282 MOTA 2115 NZ LYS 33.270 -10.495 33.583 1.00 38.11 BLGL 282 2116 LYS MOTA C 32.931 -10.251 32.429 1.00 39.52 BLGL ATOM 2117 LYS 282 0 1.00 42.82 BLGL 33.920 33.967 -11.575 2118 283 ASN MOTA N 34.355 -12.558 32.914 1.00 46.20 BLGL 2119 ASN 283 MOTA CA BLGL 1.00 50.82 283 35.290 -13.614 33.512 2120 ASN MOTA CB 1.00 56.85 BLGL 36.534 -13.010 34.122 ATOM 2121 CG ASN 283 BLGL 36.474 -12.369 35.175 1.00 61.22 ASN 283 2122 OD1 MOTA BLGL 37.672 -13.200 33.461 1.00 58.97 283 ATOM 2123 ND2 ASN 33.100 -13.246 32.163 -13.532 BLGL 1.00 45.60 32.382 283 ATOM 2124 C ASN BLGL 33.138 1.00 44.14 ATOM 2125 0 ASN 283 BLGL 284 33.081 -13.507 31.080 1.00 44.05 2126 GLY MOTA N BLGL 30.499 1.00 42.01 31.927 -14.166 MOTA 2127 CA GLY 284 BLGL 284 30.920 -13.195 29.918 1.00 40.47 GLY 2128 ATOM С 1.00 41.73 BLGL 30.072 -13.590 29.114 284 ATOM 2129 0 GLY 30.997 -11.929 BLGL 285 30.321 1.00 36.97 . 2130 ·GLN MOTA N 1.00 32.62 BLGL 29.794 285 -30.081 ->0.934 MOTA .2131 CA GLN BLGL 1.00 31.11 285 29.904 -9.781 30.771 GLN ATOM 2132 CB 1.00 29.26 BLGL 285 29.440 -10.187 32,149 MOTA 2133 CG GLN 1.00 27.08 BLGL 285 29.234 -8.985 33.046 ATOM 2134 CD GLN 29.922 1.00 26.10 BLGL -7.973 32.910 2135 285 ATOM OE1 GLN 28.296 -9.091 1.00 25.79 BLGL NE2 GLN 285 33.974 ATOM 2136 1.00 30.85 BLGL 30.634 -10.397 28.487 285 MOTA 2137 С GLN BLGL 31.844 -10.301 1.00 31.43 28.302 GLN 285 ATOM 2138 0 27.581 1.00 29.00 BLGL 286 29.735 -10.047 MOTA 2139 N THR 1.00 26.23 BLGL 286 30.119 -9.51626.292 ATOM 2140 CA THR 1.00 26.60 BLGL -9.741 286 29.000 25.280 ATOM 2141: CB THR BLGL 28.755 -11.147 25.159 1.00 26.51 ATOM 2142 OG1 THR 286 1.00 26.18 BLGL 29.370 -9.150 23.928 ATOM 2143 CG2 THR 286 -8.030 1.00 25.38 BLGL 26.413 286 30.401 ATOM 2144 С THR BLGL 286 29.553 -7.266 26.859 1.00 25.73 2145 THR ATOM 0 -7.619 1.00 25.58 BLGL 26.016 31.596 ATOM 2146 N LEU 287 BLGL 31,957 -6.219 26.098 1.00 25.95 LEU 287 ATOM 2147 CA BLGL 33,036 -6.034 27.159 1.00 23.53 287 MOTA 2148 CB LEU BLGL 1.00 22.29 2149 CG LEU 287 32.593 -6.516 28.539 ATOM 1.00 21.57 BLGL -6.413 29.523 33.742 287 ATOM 2150 CD1 LEU BLGL 1.00 20.26 2151 CD2 LEU. 287 31.409 -5.692 28.998 ATOM 1.00 28.08 BLGL -5.739 24.748 287 32.446 ATOM 2152 С LEU BLGL 1.00 29.85 2153 0 LEU 287 33.648 -5.666 24.503 ATOM 23.870 1.00 29.45 BLGL ~5.406 31.508 MOTA 2154 И ASN 288 BLGL 31.869 -4.949 22.537 1.00 31.56 ATOM 2155 CA ASN 288 21.632 1.00 35.67 BLGL -4.928 288 30.641 ATOM 2156 CB ASN BLGL 1.00 41.56 30.039 -6.306 21.456 MOTA 2157 CG ASN 288 -7.298 21.320 1.00 42.80 BLGL 30.766 ATOM 2158 OD1 ASN 288 BLGL 28.707 -6.380 21.449 1.00 43.66 ATOM 2159 ND2 ASN 288 22.523 1.00 30.88 BLGL 32.533 -3.590MOTA 2160 ASN 288 C BLGL -3.281 21.615 1.00 32.37 2161 ASN 288 33.295 ATOM O 1.00 30.69 BLGL 23.520 MOTA 2162 ASN 289 32.242 -2.767 N BLGL 23.583 1.00 29.17 289 32,849 -1.447MOTA 2163 CA ASN 23.737 1.00 29.80 BLGL 31.778 -0.364 2164 ASN 289 **ATOM** CB BLGL 22.420 1.00 34.65 ASN 289 31.108 -0.018 ATOM 2165 CG BLGL 21.529 1.00 36.80 31.733 ASN 289 0.562 ATOM 2166 OD1 BLGL 22.285 1.00 34.27 29.834 -0.382 ND2 ASN 289 MOTA 2167

Fig. 4 cont.

-1.386

-2.144

-0.497

0.459

-0.375

0.616

1.470

0.132

0.916

-0.334

24.746

25.718

24.654

23.576

25.740

25.184

24.294

27.006

26.951

28.149

1.00 28.28

1.00 26.00

1.00 26.69

1.00 25.39

1.00 24.60

1.00 23.11

1.00 24.06

1.00 25.03

1.00 24.16

1.00 23.84

BLGL

BLGL

BLGL

BLGL

BLGL

BLGL

BLGL

BLGL

BLGL

	159/174									
ATOM	2178	CA	VAL	291	35.019	0.083	29.420	1.00 21.28	BLGL	
ATOM	2179	CB	VAL	291	35.340	-0.945	30.520	1.00 21.94	BLGL	
MOTA	2180	CG1	VAL	291	34.752	-0.488	31.852	1.00 20.42	BLGL	
MOTA	2181	CG2		291	34.775	-2.309	30.114	1.00 17.11	BLGL BLGL	
MOTA	2182	C	VAL	291	35.607	1,448	29.760 30.588	1.00 20.16 1.00 19.20	BLGL	
MOTA	2183	0	VAL	291 292	36.504 35.100	1.574 2.464	29.070	1.00 19.20	BLGL	
MOTA	2184 2185	И СА	THR THR	292 292	35.532	3.842	29.250	1.00 18.74	BLGL	
MOTA MOTA	2186	CB	THR	292	36.660	4.228	28.251	1.00 18.53	BLGL	
ATOM	2187		THR	292	36.111	4.400	26.939	1.00 17.67	BLGL	
ATOM	2188	CG2	THR	292	37.716	3.148	28.196	1.00 17.15	BLGL	
ATOM .	2189	С	THR	292	34.335	4.759	28.994	1.00 19.39	BLGL BLGL	
MOTA	2190	Ο.	THR	292	33.275	4.308	28.568	1.00 19.27 1.00 20.06	BLGL . BLGL	
ATOM	2191		VAL	29 <u>3</u> 293	34.514 33.446	6.048 7.005	29.252 29.039	1.00 20.55	BLGL	
MOTA	2192 2193	CA CB	VAL VAL	293	33.865	8.406	29.544	1.00 20.16	BLGL	
ATOM ATOM	2193		VAL	293	32.857	9.451	29.100	1.00 20.66	BLGL	
ATOM	2195		VAL	293	33.936	8.390	31.074	1.00 16.78	BLGL	
ATOM	2196	С	VAL	293	33.051	7.044	27.562	1.00 20.97	BLGL	
MOTA	2197	<b>O</b> .	VAL	293	31.864	7.124	27.234	1.00 21.53	BLGL	
MOTA	2198	N	GLN	294	34.039	6,962	26.674	1.00 20.45 1.00 21.64	BLGL BLGL	
ATOM	2199	CA	GLN	294	33.770	6.956 7.058	25.238 24.431	1.00 21.64	BLGL	
ATOM	2200 2201	CB.	GLN GLN	294 294	35.066 35.192	8.341	23.619	1.00 29.52	BLGL	
ATOM ATOM	2201	CD	GLN	294	34.031	8.562	22.666	1.00 29.94	BLGL	
ATOM	2203		GLN	294	33.739	9.696	22.296	1.00 34.05	BLGL	
ATOM	2204	NE2		294	33.371	7.485	22.260	1.00 28.56	BLGL	
ATOM	2205	С	GLN	294	33.058	5.672	24.834	1.00 22.39	BLGL	
MOTA	2206	0	GLN	294	32.199	5.677	23.950	1.00 19.94	BLGL BLGL	
ATOM-	2207	N	GLY	295	33.444	4.566 3,295	25.468 25.173	1.00 22.59 1.00 20.59	BLGL	
ATOM	2208	CA	GLY GLY	295 295	32.814 31.349	3.362	25.564	1.00 22.43	BLGL	
МОТА МОТА	2209 2210	C O	GLY	295	30.464	3.047	24.767	1.00 23.22	BLGL	
ATOM	2211	N	GLN	296	31.099	3.787	26.798	1.00 19.02	BLGL	
ATOM	2212	CA	GLN	296	29.750	3.905	27.313	1.00 19.21	BLGL	
ATOM	2213	CB	GLN	296	29.789	4.581	28.683	1.00 19.90	BLGL	
ATOM	2214	CG	GLN	296	28.467	4.668	29.419	1.00 18.48	BLGL BLGL	
ATOM	2215	CD	GLN	296	28.572	5.536	30.669 30.595	1.00 17.80 1.00 16.03	BLGL	
MOTA	2216		GLN GLN	296 296	29.027 28.152	6.679 4.999	31.818	1.00 15.03	BLGL	
MOTA MOTA	2217 2218	C	GLN	296	28.906	4.719	26.336	1.00 19.79	BLGL	
ATOM	2219	Ö	GLN	296	27.777	4.347	26.016	1.00 20.36	BLGL	
ATOM	2220	N	ALA	297	29.458	5.825	25.851	1.00 18.99	BLGL	
ATOM	2221	CA	ALA	297	28.733	6.669	24.905	1.00 18.45	BLGL	
ATOM	2222	CB	ALA	297	29.546	7.916	24.578	1.00 14.36	BLGL BLGL	
ATOM	2223	C	ALA	297	28.416 27.301	5.895 5.978	23.630 23.104	1.00 19.50 1.00 20.34	BLGL	
ATOM ATOM	2224 2225	0	ALA ASN	297 298	29.395	5.142	23.135	1.00 19.83	BLGL	
ATOM	2225	CA	ASN	298	29.196	4.352	21.926	1.00 21.45	BLGL	
MOTA	2227	СВ	ASN	298	30.442	3.524	21.592	1.00 24.97	BLGL	
ATOM	2228	ÇĞ	ASN	298	31.563	4.358	20.999	1.00 26.63	BLGL	
MOTA	2229		. ASN	298	31.329	5.440	20.459	1.00 25.65	BLGL	
MOTA	2230		ASN	298	32.791	3.843	21.078	1.00 27.74	BLGL BLGL	
MOTA	2231	C	ASN	298	28.027	3.405	22.133 21.297	1.00 21.39 1.00 21.38	BLGL	
MOTA	2232	0	ASN		27.130 28.061	3.306 2.713	23.266	1.00 19.25	BLGL	
MOTA MOTA	2233 2234	N CA	ALA ALA		27.038		23.633		BLGL	
ATOM	2234	CB	ALA		27.294	1.264	25.030	1.00 16.35	BLGL	
ATOM	2236	c	ALA		25.638	2.339	23.537	1.00 19.35	BLGL	
ATOM	2237	Ö	ALA	299	24.763	1.771	22.881	1.00 17.73	BLGL	
ATOM	2238	N	VAL		25.432		24.201		BLGL	
ATOM	2239	CA	VAL		24.134				BLGL BLGL	
MOTA	2240	CB CC1	VAL		24.141 22.786				BLGL	
ATOM ATOM	2241 2242		VAL VAL		24.467				BLGL	
ATOM	2242	C	VAL		23.761	4.597			BLGL	

Fig. 4 cont.

	160/174										
ATOM	2244	0	VAL	300	22.643	4.383	22.332	1.00 22.02	BLGL		
ATOM	2245	N	ARG	301	24.711	5.220	22.117	1.00 19.80	BLGL		
MOTA	2246	CA	ARG	301	24.485	5.699	20.770	1.00 20.87 1.00 20.72	BLGL BLGL		
MOTA	2247	CB	ARG	301	25.764	6.370 6.960	20.273 18.884	1.00 20.72	BLGL		
ATOM	2248	CG	ARG	301 301	25.697 25.963	5.909	17.841	1.00 20.20	BLGL		
ATOM ATOM	2249 2250	CD NE	ARG ARG	301	25.950	6.479	16.502	1.00 21.66	BLGL		
ATOM	2251	CZ	ARG	301	25.770	5.763		1.00 21.05	BLGL		
ATOM	2252	NH1		301	25.593	4.453	15.484	1.00 23.39	BLGL		
ATOM	2253	NH2	ARG	301	25.741	6.359	14.223	1.00 19.98	BLGL		
ATOM	2254	С	ARG	301	24.050	4.575	19.824	1.00 21.51	BLGL BLGL		
MOTA	2255	0	ARG	301	23.190	4.774 3.394	18.967 19.989	1.00 23.05 1.00 20.34	BLGL		
ATOM	2256	N	ASP	302 302	24.633 24.306	2.262	19.138	1.00 20.34	BLGL		
ATOM ATOM	2257 2258	CA CB	ASP	302	25.378	1.190	19.260	1.00 22.07	BLGL		
ATOM	2259	CG	ASP	302	26.659	1.571	18.548	1.00 26.74	BLGL		
MOTA	2260		ASP	302	27.647	0.818	18.676	1.00 31.70	BLGL		
MOTA	2261	OD2	ASP	302	26.686	2.618	17.857	1.00 28.72	BLGL		
MOTA	2262	C.	ASP	302	22.947	1.648	19.408	1.00 20.74	BLGL BLGL		
MOTA	2263	0	ASP	302	22.329	1.083	18.509 20.644	1.00 23.13 1.00 18.00	BLGL		
MOTA	2264	N	VAL VAL	303 303	22.482 21.182	1.740 1.189	20.971	1.00 18.00	BLGL		
MOTA MOTA	2265 2266	CA CB	VAL	303	20.971	1.110	22.503	1.00 17.67	BLGL		
ATOM	2267		VAL	303	19.626	0.483	22.813	1.00 17.30	BLGL		
ATOM	2268		VAL	303	22.075	0.299	23.132	1.00 20.13	BLGL		
ATOM	.2269	С	VAL	303	20.126	2.099	20.346	1.00 18.76	BLGL		
MOTA	2270	0	VAL	303	19.099	1.638	19.854	1.00 16.54	BLGL.		
MOTA	2271	N	ILE	304	20.392	3.401 4.371	20.367 19.793	1.00 19.37 1.00 20.60	BLGL		
MOTA	2272	CA	ILE	304 304	19.471 19.955	5.820	20.067	1.00 20.00	BLGL		
ATOM ATOM	2273 _. 2274	CB	ILE	.304	19.113	6.835	19.293	1.00 19.25	BLGL		
ATOM	2275		ILE	304	19.853	6.108	21.567	1.00 21.33	BLGL		
ATOM	2276		ILE	304	20.334	7.482	21.961	1.00 21.10	BLGL		
ATOM	2277	С	ILE	304	19.387	4.102	18.294	1.00 21.62	BLGL		
MOTA	2278	0	ILE	304	18.316	4.130	17.695	1.00 22.05	BLGL		
MOTA	2279	N	GLN	305	20.531	3.820 3.523	17.694 16.279	1.00 21.95 1.00 22.70	BLGL BLGL		
ATOM	2280	CA	GLN GLN	305 305	20.579 22.031	3.274	15.855	1.00 25.34	BLGL		
ATOM ATOM	2281 2282	CB CG	GLN	305	22.203	2.958	14.381	1.00 28.30	BLGL		
ATOM	2283	CD	GLN	305	22.031	4.178	13.505	1.00 30.27	BLGL		
ATOM	2284		GLN'	305	22.915	5.030	13.430	1.00 30.12	BLGL		
MOTA	2285	NE2	GLN	305	20.884	4.273	12.841	1.00 32.34	BLGL		
ATOM	2286	С	GLN	305	19.736	2.278	16.006	1.00 22.92 1.00 23.46	BLGL BLGL		
MOTA	2287	0	GLN	305	18.925 19.931	2.258 1.247	15.080 16.831	1.00 23.48	BLGL		
ATOM ATOM	2288 2289	N CA	ALA ALA	306 306	19.331	-0.031	16.693	1.00 21.78	BLGL		
ATOM	2290	CB	ALA	306	19.708	-1.019	17.743	1.00 18.27	BLGL		
ATOM	2291	c	ALA	306	17.704	0.090	16.773	1.00 22.33	BLGL		
ATOM	2292	0	ALA	306	16.987	-0.569	16.018	1.00 23.37	BLGL		
ATOM	2293	N	VAL	307	17.219	0.919		1.00 20.00	BLGL		
MOTA	2294	CA	VAL	307	15.788	1.112	17.844	1.00 20.55	BLGL BLGL		
ATOM	2295	CB	VAL	307	15.450	1.823 2.106		1.00 20.50 1.00 17.36	BLGL		
ATOM ATOM	2296 2297		VAL VAL	307 307	13.959 15.878	0.960		1.00 17.55	BLGL		
ATOM	2298	C	VAL	307	15.274	1.959			BLGL		
ATOM	2299	Ö	VAL	307	14.164	1.750			BLGL		
ATOM	2300	N	SER	308	16.097	2.916			BLGL		
ATOM	2301	CA	SER	308	15.750	3.818			BLGL		
MOTA	2302	CB	SER	308	16.809	4.916			BLGL		
ATOM	2303	OG	SER	308	16.510	5.812			BLGL BLGL		
MOTA	2304	C	SER	308	15.633	3.059 3.372			BLGL		
MOTA ATOM	2305 2306	о И	SER ASP	308 309	14.781 16,490	2.057			BLGL		
MOTA	2306	CA	ASP	309	16.480	1.252		1.00 23.50	BLGL		
ATOM	2308	СВ	ASP	309	17.698	0.332		1.00 25.27	BLGL		
ATOM	2309	CG	ASP	309	18.971	1.069	12.064	1.00 29.05	BLGL		
							-				

Fig. 4 cont.

### 161/174 2.130 11,401 1.00 26.38 BLGL 18.874 309 2310 OD1 ASP ATOM 0.576 BLGL 20.066 12.423 1.00 30.01 309 OD2 ASP ATOM 2311 12.339 1.00 24.33 BLGL 309 15.225 0.412 ASP MOTA 2312 C BLGL 14.972 -0.12411.265 1.00 26.71 309 ASP ATOM 2313 0 13.409 1.00 24.29 BLGL 14.450 0.280 310 VAL ATOM 2314 N -0.490 13.344 1.00 23.62 BLGL VAL 310 13.219 MOTA 2315 CA 1.00 23.06 BLGL -0.647 14.730 310 12.582 VAL MOTA 2316 CB--1.336 14.606 1.00 21.23 BLGL CG1 VAL 310 11.232 MOTA 2317 310 13.509 -1.443 15.632 1.00 21.91 BLGL CG2 VAL ATOM 2318 1.00 23.63 12.440 BLGL 0.247 MOTA 2319 С VAL 310 12,248 -0.352 11.834 1.00 25.38 BLGL 11.360 310 VAL MOTA 2320 0 12.343 1.00 23.71 BLGL 1.555 MOTA 2321 N GLY 311 12.438 11.519 1.00 23.98 BLGL 11.573 2.373 CA GLY 311 MOTA 2322 1.00 27.47 BLGL 3.201 12.366 ATOM 2323 С GLY 311 10.628 3.565 13.514 1.00 28.40 BLGL 10.919 311 MOTA 2324 0 GLY BLGL 1.00 27.49 11.783 2325 N GLU 312 9.469 3.474 ATOM 4.262 12.419 1.00 27.36 BLGL 8.438 ATOM 2326 CA GLU 312 BLGL 1.00 32.86 7.210 4.291 11.514 2327 CB GLU 312 ATOM 5.503 11.705 1.00 43.92 BLGL 6.318 2328 GLU 312 MOTA CG BLGL 1.00 50.44 5.314 11.071 2329 CD GLU 312 4.950 ATOM BLGL 4.889 9.930 1.00 51.60 4.793 2330 OE1 GLU 312 ATOM BLGL 5.694 11.713 1.00 53.86 OE2 GLU 312 3.939 ATOM 2331 3.746 BLGL 8.039 13.805 1.00 25.87 ATOM 2332 C GLU 312 BLGL 1.00 27.15 4.537 14.683 GLU 312 . 7.717 ATOM 2333 O BLGL 8.067 2.431 14.003 1.00 22.50 2334 N ALA 313 MOTA BLGL 7.671 1.814 15.273 1.00 19.75 2335 CA ALA 313 ATOM BLGL 7.480 15.077 1.00 19.28 0.315 ATOM 2336 CB ALA 313 BLGL 8.608 2.054 16.454 1.00 18.86 ALA 313 MOTA 2337 C 2.049 17.602 BLGL 1.00 15.56 2338 ALA 313 8.167 MOTA 0 BLGL 9.897 2.238 16.173 1,00 19.40 2339 GLY 314 ATOM N 17.232 1.00 21.12 BLGL 2340 ĊA GLY 314 10.868 2.476 ATOM BLGL 3.878 17.787 1.00 22.30 C GLY 314 10.667 ATOM 2341 17.135 1.00 23.19 BLGL 2342 GLY 314 11.016 4.865 ATOM 10.122 3.973 18.997 1.00 19.98 BLGL ILE 315 2343 N ATOM 1.00 18.06 19.580 BLGL 5.267 ATOM 2344 CA ·ILE 315 9.841 5.265 20.248 1.00 17.92 BLGL 8.457 CB ILE 315 MOTA 2345 1.00 16.03 BLGL 19.221 7.402 4.928 MOTA 2346 CG2 ILE 315 CG1 ILE 8.417 4.242 21.378 1.00 17.81 BLGL 315 ATOM 2347 BLGL 1.00 16.57 22.116 4.236 ATOM 2348 CD1 ILE 315 7.113 BLGL 10.852 5.818 20.563 1.00 18.49 315 2349 C ILE MOTA 1.00 19.85 BLGL 7.012 20.836 2350 315 10.851 MOTA O ILE 11.719 4.974 21.101 1.00 18.64 BLGL MOTA 2351 GLY 316 N BLGL 1.00 17.78 22.042 12.692 5.492 ATOM 2352 ÇA GLY 316 13.562 1.00 18.38 BLGL 4.510 22.803 GLY MOTA 2353 C 316 BLGL 1.00 17.99 22.618 MOTA 2354 0 GLY 316 13.500 3.290 1.00 17.69 BLGL VAL 317 14.381 5.081 23.680 MOTA 2355 N 1.00 17.45 BLGL 24.512 317 15.312 4.328 ATOM 2356 CA VAL BLGL VAL 317 16.727 4.367 23.916 1.00 17.12 ATOM 2357 CB 1.00 16.69 BLGL 24.882 17.710 3.738 ATOM 2358 CG1 VAL 317 22.586 1.00 16.13 BLGL 16.753 3.642 CG2 'VAL 317 ATOM 2359 1.00 17.08 BLGL 15.385 4.902 25.921 MOTA 2360 С VAL 317 1.00 19.09 BLGL 6.116 26.101 317 15.386 **ATOM** 2361 0 VAL BLGL 1.00 17.11 15.441 4.032 26.920 PHE 318 ATOM 2362 N 4.488 BLGL 15.547 28.298 1.00 16.85 ATOM 2363 CA PHE 318 1.00 17.66 BLGL 14.389 3.976 29.146 CB PHE 318 ATOM 2364 BLGL 29.068 1.00 19.59 13.154 4.821 MOTA 2365 CG PHE 318 12.208 4.615 28.063 1.00 17.88 BLGL CD1 PHE 318 MOTA 2366 30.017 BLGL 1.00 18.14 MOTA 2367 CD2 PHE 318 12.922 5.811 11.041 28.007 1.00 15.40 BLGL CE1 PHE 318 5.383 ATOM 2368 BLGL 6.585 29.968 1.00 20.01 11.760 MOTA 2369 CE2 PHE 318

Fig. 4 cont.

6.367

3.996

2.802

4.914

4.531

5.676

10.815

16.839

17.132

17.619

18.859

19.876

CZ

С

0

N

ĊA

CB

2370

2371

2372

2373

2374

2375

ATOM

ATOM

MOTA

MOTA

ATOM

MOTA

PHE

PHE

PHE

TYR

TYR

TYR

318

318

318

319

319

319

28.960

28.914

28.878

29.471

30.127

30.103

1.00 16.53

1.00 17.63

1.00 19.56

1.00 17.12

1.00 17.31

1.00 15.56

BLGL

BLGL

BLGL

BLGL

BLGL

					16	2/174			
ATOM	2376	CG	TYR	319	21,255	5.211	30.495	1.00 17.60	BLGL
ATOM	2377	CD1		319	22.257	5.060	29.541	1.00 16.51	BLGL
ATOM	2378	CE1	TYR	319	23.503	4.568	29.886	1.00 17.94	BLGL
ATOM	2379	CD2		319	21.541	4.860	31.815	1.00 17.35 1.00 18.20	BLGL BLGL
MOTA	2380	CE2		319	22.781	4.366 4.220	32.174 31.207	1.00 18.82	BLGL
MOTA	2381	CZ	TYR	319 319	23.761 24.993	3.717	31.560	1.00 17.43	BLGL
ATOM ATOM	2382 2383	-C OH	TYR TYR	319	18.465	4.214	31.568	1.00 15.84	BLGL
ATOM	2384	Ö	TYR	319	17.852	5.040	32.231	1.00 17.43	BLGL
ATOM	2385	N	TRP	320	18.811	3.024	32.050	1.00 15.86	BLGL
ATOM	2386	CA	TRP	320	18.448	2.622	33,408	1.00 14.37	BLGL
ATOM	2387	СВ	TRP	320	18.286	1.099	33.489	1.00 13.03 1.00 13.67	BLGL BLGL
ATOM	2388	CG	TRP	320	17.673 18.348	-0.644 -0.001	34.786 35.873	1.00 13.63	BLGL
MOTA	2389 2390		TRP	320 320	17.408	-0.123	36.930	1.00 16.14	BLGL
ATOM ATOM	2391		TRP	320	19.654	÷0.480	36.063	1.00 12.95	BLGL
ATOM	2392		TRP	320	16.388	0.865	35.210	1.00 10.20	BLGL
ATOM	2393		TRP	320 .	16.225	0.413	36.491	1.00 11.94	BLGL
MOTA	2394		TRP	320	17.736	-0.706	38.171	1.00 14.00	BLGL BLGL
MOTA	2395		TRP:	320	19.984	71.057	37.292 38.332	1.00 14.81 1.00 15.77	BLGL
MOTA	2396	CH2		320	19.023 19.428	-1.163 3.071	34.484	1.00 13.77	BLGL
ATOM	2397 2398	C O	TRP TRP	320 320	20.624	2.786	34.403	1.00 13.40	BLGL
MOTA MOTA	2399	N	GLÜ	321	18.898	3.770	35.487	1.00 14.52	BLGL
ATOM	2400	CA	.GLU	321	19.671	4.261	36.630	1.00 16.07	
ATOM	.2401	СВ	GLU	321	19.878	3.117	37.634	1.00 16.50	BLGL
ATOM	2402	CG	GLU	321	18.605	2.675	38.362	1.00 15.22	BLGL
MOTA	2403	CD	GLU	321	18.179		39.439 40.156	1.00 15.33 1.00 13.74	BLGL BLGL
MOTA	2404		GLU	321	17.190 18.840	3.375 4.703	39.573	1.00 13.74	BLGL
ATOM ATOM	2405 2406	C	GLU GLU	321 321	21.015	4.890	36.267	1.00 16.30	BLGL
ATOM	2407	Ö	GLU	321	22.078	4.321	36.533	1.00 19.88	BLGL
ATOM	2408	N	PRO	322	20.985		35.664	1.00 13.95	BLGL
ATOM	2409	CD	PRO	322	19.800	6.807	35.166	1.00 13.71	BLGL
MOTA	2410	CA	PRO	322	22.207	6.776	35.269	1.00 13.32	BLGL
MOTA	2411	CB	PRO	322	21.727	7.665	34.136	1.00 13.68 1.00 11.78	BLGL BLGL
ATOM	2412	CG	PRO PRO	322 322	20.397 22.8 <u>2</u> 6	8.108 7.588	34.648 36.391	1.00 14.16	BLGL
MOTA MOTA	2413 2414	С 0	PRO	322	23.849	8.235	36.191	1.00 17.47	BLGL
ATOM	2415	N	ALA	323	22.215	7.564	37.568	1.00 12.38	BLGL
ATOM	2416	CA	ALA	323	22.742	8.345	38.676	1.00 11.98	BLGL
MOTA	2417	CB	ALA	323	21.979	9.660	38.786	1.00 8.04	BLGL
ATOM	2418	С	ALA	323	22.736	7.619	40.012	1.00 12.24	BLGL BLGL
ATOM	2419	0	ALA	323	22.580 22.910	8.245 6.300	41.060 39.980	1.00 10.35	BLGL
ATOM ATOM	2420 2421	N CA	TRP TRP	324 324	22.933	5.515	41.215	1.00 15.62	BLGL
ATOM	2422	CB	TRP	324	22.422	4.094	40.973	1.00 15.22	BLGL
ATOM	2423	CG	TRP	324	21.843	3.473	42.201	1.00 16.28	BLGL
ATOM	2424		TRP	324	20.827	2.465	42.257	1.00 18.02	BLGL
ATOM	2425		TRP	324	20.595	2.181	43.622	1.00 18.70	BLGL
ATOM	2426		TRP	324	20.086	1.776		1.00 16.37	BLGL BLGL
MOTA	2427		LTRP	324	22.178 21.434	3.748 2.978		1.00 17.37	BLGL
MOTA	2428 2429		L TRP	324 324	19.655	1.231	44.044	1.00 19.78	BLGL
MOTA MOTA	2429		3 TRP	324	19.154	0.834	41.703	1.00 16.22	BLGL
MOTA	2431		2 TRP	324	18.944	0.570	43.071	1.00 18.68	BLGL
ATOM	2432	С	TRP	324	24.378	5.467	41.707		BLGL
ATOM	2433	0	TRP		24.986	4.405			BLGL
ATOM	2434	N	ILE	325	24.916	6.645			BLGL BLGL
MOTA	2435	CA	ILE		26.284	6.781			BLGL
MOTA	2436	CB	ILE		26.796 26.652	8.203 8.518			BLGL
ATOM ATOM	2437 2438		2 ILE 1 ILE		26.021	9.212			BLGL
ATOM	2439		1 ILE		26.493	10.630	42.843	1.00 14.92	BLGL
ATOM	2440	C	ILE		26.448	6.429	43.926	1.00 21.37	BLGL
ATOM	2441	0	ILE		25.473	6.373	44.675	1.00 20.25	BLGL
						-	4		

Fig. 4 cont.

ATOM

2507

OE2 GLU

163/174 BLGL 1.00 22.85 27.697 6.188 44.358 ATOM 2442 N PRO 326 43.557 1.00 21.92 BLGL 28.935 6.258 326 MOTA 2443 CD PRO BLGL 27.988 5.827 45.750 1.00 23.11 MOTA 2444 CA PRO 326 45.724 1.00 21.79 BLGL 29.488 5.535 2445 PRO 326 MOTA CB 1.00 23.00 BLGL 29.992 6.401 44.613 2446 PRO 326 MOTA CG 27.604 6.851 46.806 1.00 22.87 BLGL 326 PRO C MOTA 2447 BLGL 46.564 1.00 22.51 27.666 8.055 ATOM 2448 0 PRO 326 1.00 22.78 BLGL 6.360 47.975 27.189 VAL 327 ATOM 2449 N 49.083 1.00 24.67 BLGL 26.812 7.236 MOTA 2450 CA VAL 327 327 25.918 6.519 50.133 1.00 26.26 BLGL VAL CB ATOM 2451 BLGL 49.478 1.00 27.07 24.651 5.996 ATOM 2452 CG1 VAL 327 1.00 23.81 BLGL 327 26.691 5.393 50.805 VAL 2453 CG₂ MOTA 49.798 1.00 25.35 BLGL 28.072 7.697 2454 VAL 327 ATOM C BLGL 327 28.036 8.643 50.582 1.00 25.02 VAL ATOM 2455 0 1.00 26.68 BLGL 49.516 GLY 328 29.176 7.007 MOTA 2456 N 50.120 BLGL 328 30.459 7.315 1.00 27.54 2457 GLY ATOM CA 1.00 29.31 BLGL 49.551 ATOM 2458 С GLY 328 31.540 6.412 48.938 1.00 29.16 BLGL 328 31.219 5.392 GLY MOTA 2459 0 49.743 1.00 30.18 BLGL 6.751 2460 329 32.830 N PRO MOTA 1.00 30.73 BLGL PRO 329 33.277 7.948 50.477 ATOM 2461 CD 49.255 1.00 30.09 BLGL 329 33.989 5.994 2462 PRO MOTA CA 6.722 1.00 30.88 BLGL 35.166 49.891 PRO 329 MOTA 2463 CB 1.00 31.43 BLGL 49.959 2464 CG PRO 329 34.685 8.128 ATOM 49.614 1.00 29:93 BLGL 33.966 4.520 329 MOTA 2465 С PRO 50.639 1.00 30.03 BLGL 329 33.416 4.132 2466 О PRO MOTA 3.706 48.768 1.00 29.86 BLGL 330 34.582 ATOM 2467 . N ALA BLGL 48.987 1.00 32.93 330 34.614 2.272 ATOM 2468 CA ALA 47.833 1.00 31.50 BLGL 35.343 1.585 MOTA 2469 CB ALA 330 1.00 35.35 BLGL 330 35.265 1.911 50.313 2470 С ALA ATOM 1.00 35.56 BLGL 34.894 0.916 50.940 330 ATOM 2471 0 ALA BLGL 1.00 37.94 331 36.228 2.721 50.749 2472 Ν . HIS ATOM 1.00 40.82 BLGL 36.922 2.440 52.001 331 MOTA 2473 CA HIS BLGL 38.282 3.143 52.049 1.00 41.19 MOTA 2474 CB HIS 331 1.00 42.83 BLGL 52.171 38.195 4.632 MOTA 2475 CG HIS 331 1.00 42.69 BLGL 2476 CD2 HIS 331 38.170 5.436 53.261 ATOM 5.469 1.00 43.41 BLGL 51.077 38.130 MOTA 2477 ND1 HIS 331 BLGL 51.488 1.00 42.26 2478 CE1 HIS 331 38.073 6.725 MOTA 38.096 6.732 52.809 1.00 42.43 BLGL 331 ATOM 2479 NE2 HIS 1.00 42.32 BLGL ATOM 2480 C HIS 331 36.130 2.805 53.254 2.788 36.674 54.354 1.00 43.73 BLGL 331 ATOM 2481 O HIS 1.00 43.54 53.105 BLGL 34.857 3.149 ATOM 2482 N ARG 332 34.041 54.264 1.00 43.67 BLGL ARG 332 3.478 ATOM 2483 CA BLGL 1.00 46.16 33.446 4.878 54.152 2484 CB ARG 332 ATOM BLGL 34.428 54.232 1.00 51.93 6.031 ATOM 2485 ARG 332 CG 1.00 55.92 BLGL ARG 332 33.693 7.258 54.754 ATOM 2486 CD BLGL 7.299 54.240 1.00 62.04 32,323 2487 ARG 332 ATOM NE BLGL 1.00 64.85 31.376 8.138 54.664 ARG 332 ATOM 2488 CZBLGL 30.154 8.095 54.132 1.00 64.81 ATOM 2489 NH1 ARG 332 BLGL 1.00 65.83 31.640 9.023 55.622 2490 332 ATOM NH2 ARG BLGL 54.368 1.00 43.46 32.899 2.482 ATOM 2491 ARG 332 С 1.00 42.10 BLGL 31.882 2.766 54.999 ARG 332 2492 a ATOM BLGL 53.748 1.00 43.54 33.077 1.318 **ATOM** 2493 N LEU 333 1.00 44.90 BLGL 32.058 0.277 53.739 LEU 333 2494 CA MOTA 32.700 -1.104 53.605 1.00 44.71 BLGL 2495 CB LEU 333 MOTA BLGL 52.511 1.00 47.14 LEU 333 32.076 -1.981ATOM 2496 CG BLGL 52.561 1.00 47.53 2497 PEA 333 32.702 -3.370 ATOM CD1 30.561 52.691 1.00 46.62 BLGL -2.068 CD2 LEU 333 2498 MOTA 1.00 46.15 BLGL 54.959 MOTA 2499 С LEU 333 31.154 0.282 1.00 47.20 BLGL 29.931 0.378 54.833 2500 LEU 333 ATOM 0 BLGL 1.00 47.86 56.139 MOTA 2501 Ŋ GLU 334 31.755 0.183 0.159 1.00 48.83 BLGL 30.989 57.384 ATOM 2502 CA GLU 334 BLGL 1.00 51.92 2503 GLU 334 31.934 0.012 58.584 MOTA CB 58.641 1.00 58.71 BLGL 32.639 -1.345MOTA 2504 CG GLU 334 BLGL 1,00 61.85 31.663 -2.521 58.588 ATOM 2505 CD GLU 334 -2.642 59.510 1.00 62.23 BLGL 30.824 ATOM 2506 OE1 GLU 334 1.00 63.86 BLGL 57.622 31.734 334 -3.319

Fig. 4 cont.

					16	4/174				
MOTA	2508	С	GLU	334	30.083	1.374	57.584	1.00		BLGL
ATOM	2509		GLU	334	28.939	1.246	58.030	1.00		BLGL
MOTA	2510	N	LYS	335	30.583	2.552 3.752	57.251 57.415	1.00		BLGL BLGL
MOTA	2511	CA	LYS LYS	335 335 ·	29.783 30.687	4.980	57.370	1.00		BLGL
MOTA MOTA	2512 2513	CB CG	LYS	335	30.158	6.168	58.168	1.00		BLGL
MOTA	2514	CD	LYS	335	29.958	5.809	59.653	1.00		BLGL
MOTA	2515	CE	LYS	335	31.207	5.161	60.270	1.00		BLGL
ATOM	2516	NZ	LYS	335	32.440	5.982 3.843	60.078 56.318	1.00		BLGL BLGL
ATOM	2517 2518	C	LYS LYS	335 335	28.717 27.664	4.458	56.508	1.00		BLGL
ATOM ATOM	2519	O N	ASN	336	28.999	3.229	55.169		40.89	BLGL
ATOM	2520	CA	ASN	336	28.068	3.233	54.050		36.25	BLGL
ATOM	2521	. CB	ASN	336	28.758	2.764	52.774	.1.00		BLGL
MOTA	2522	CG	ASN	336	29.754	3.770 4.949	52.252 52.593		33.73 33.95	BLGL BLGL
ATOM	2523		ASN	336 336	29.698 30.661	3.316	51.401		34.13	BLGL
ATOM ATOM	2524 · 2525	ND2	ASN	336	26.883	2.332	54.333		35.83	. BLGL .
ATOM	2526	ŏ	ASN	336	25.742	2.702	54.050		35.07	BLGL
ATOM	2527	N	LYS	337	27:161	1.147	54.882		34.86	BLGL
MOTA	2528	ĊA	ĻYS	337	26.116	0.171	55.209		33.18 31.58	BLGL BLGL
ATOM	2529	CB	LYS	337	26.712	-1.023 -1.901	55.953 55.095		32.46	BLGL
	· 2530 2531	CG CD	LYS LYS	337 337 ·	27.594 28.112	-3.095	55.881		33.49	BLGL
ATOM ATOM	2531	CE	LYS	337	28.869	-4.046	54.967	1.00	38.20	BLGL
ATOM	2533	NZ	LYS	337	29.366	-5.262	55.679		41.08	BLGL
ATOM	2534	С	LYS	337	25.042	0.812	56.069		32.37	BLGL
ATOM	2535	0	<b>LYS</b>	337	23.866	0.477	55.971		30.10 32.27	BLGL BLGL
ATOM	2536	N	ALA	33B	25.466	1.738 2.434	56.917 57.793		32.10	BLGL
ATOM ATOM	2537 2538	CA CB	ALA ALA	338 338	. 24.543 25.313	3.383	58.712		30.46	BLGL
ATOM	2539	C	ALA	338	23.533	3.211	56.951	1.00	31.53	BLGL
ATOM	2540	ō	ALA	338	22.332	3.174	57.217		32.87	BLGL
MOTA	2541	N	LEU	339	24.025	3.915	55.937	1.00	29.75	BLGL
MOTA	2542	CA	LEU	339	23.165	4.703 5.580	55.064 54.149		28.75 29.58	BLGL BLGL
MOTA	2543	CB CG	LEU	339 339	24.019 24.839	6.671	54.149		29.29	BLGL
ATOM ATOM	2544 2545		LEU	339	25.763	7.358	53.858		30.28	BLGL
ATOM	2546		LEU	339	23.889	7.674	55.457		30.12	BLGL
ATOM	2547	С	LEU	339	22.246	3.824	54.217		28.58	BLGL
ATOM	2548	0	PEA	339	21.035	4.049	54.154		28.13	BLGL BLGL
MOTA	2549	N	TRP	340 340	22.828 22.052	2.828 1.925	53.557 52.719		27.39 26.49	BLGL
ATOM ATOM	2550 2551	CA CB	TRP TRP	340	22.900	0.746	52.236		23.72	BLGL
MOTA	2552	CG	TRP	340	24.091	1.114	51,444	1.00	22.86	BLGL
MOTA	2553		TRP	340	25.305	0.366	51.336		23.48	BLGL
ATOM	2554		TRP	340	26.154	1.077	50.458		23.45 23.20	BLGL BLGL
ATOM	2555		TRP	340	25.760 24.243	-0.839 2.214	51.895 50.651		22.87	BLGL
ATOM ATOM	2556 2557		TRP	340 340	25.480	2.213			22.68	BLGL
ATOM	2558		TRP	340	27.437	0.626			23.93	BLGL
MOTA	2559		TRP	340	27.036	-1.288			24.91	BLGL
ATOM	2560	CHZ	TRP	340	27.859	-0.553			23.29	BLGL
MOTA	2561	С	TRP	340	20.891	1.359		1.00	26.35 26.95	BLGL BLGL
MOTA	2562	0	TRP	340	19.777 21.179	1.252 0.990			27.03	BLGL
ATOM ATOM	2563 2564	N CA	GTN GTN	341 341	20.206	0.383			27.61	BLGL
ATOM	2565	СВ	GLU	341	20.939	-0.239			29.81	BLGL
ATOM	2566	CG	GLU	341	20.338	-1.534	57.345	1.00	32.17	BLGL
MOTA	2567	CD	GLU	341	20.490	-2.693			34.50	BLGL
ATOM	2568		GLU	341	20.087	-3.811			38.21	BLGL BLGL
MOTA	2569		2 GLU	341	21.003 19.150	-2.503 1.366			35.23 27.16	BLGL
MOTA	2570 2571	0	GLU GLU	341 341	17.967	1.044			27.02	BLGL
ATOM ATOM	2572	И	THR		19.569	2.572		1.00	27.11	BLGL
ATOM	2573	CA	THR	342	18.624	3.562			27.99	BLGL
							4			

Fig. 4 cont.

					16	5/174			
ATOM	2574	СВ	THR	342	19.356	4.706	57.658	1.00 27.99	BLGL
ATOM	2575	OG1		342	20.097	4.174	58.759	1.00 29.52	BLGL
MOTA	2576	CG2		342	18.365	5.731	58.173	1.00 28.27	BLGL BLGL
MOTA	2577	Ċ	THR	342	17.732	4.169	55.860 56.047	1.00 27.72 1.00 27.61	BLGL
ATOM	2578	0	THR	342 343	16.527 18.319	4.263	54.732	1.00 27.61	BLGL
ATOM	2579 2580	n Ca	TYR TYR	343	17.544	5.185	53.675	1.00 29.90	BLGL
ATOM ATOM	2581	CB	TYR	343	18.260	6.448	53.209	1.00 31.83	BLGL
ATOM	2582	CG	TYR	343	18.573	7.381	54.350	1.00 35.78	BLGL
ATOM	2583	CD1		343	19.798	7.313	55.013	1.00 36.95	BLGL
MOTA	2584	CE1		343	20.078	8.151	56.085	1.00 38.42	BLGL
ATOM	2585	CD2		343	17.631	8.313	54.792	1.00 35.14	BLGL BLGL
ATOM	2586	CE2		343	17.901 19.128	9.153 9.067	55.864 56.503	1.00 36.75 1.00 38.36	BLGL
ATOM ATOM	2587 2588	CZ OH	TYR TYR	343 343	19.417	9.904	57.554	1.00 40.88	BLGL
MOTA	2589	c c	TYR	343	17.202	4.327	52.469	1.00 28.69	BLGL
ATOM	2590	ō	TYR	343	16.524	4.788	51.554	1.00 28.30	BLGL
ATOM .	2591	N	GLY	344	17.652	3.081	52.470	1.00 28.37	BLGL
· ATOM	2592	CA	GLY	344	17.375	2.204	51.347	1.00 29.03	BLGL
ATOM	2593	С	GLY	344	18.001	2.730	50.068	1.00 28.56 1.00 27.04	BLGL '
MOTA	2594	0	GLY	344	17.425 19.187	2.603 3.320	48.987 50.199	1.00 27.04	BLGL
MOTA MOTA	2595 2596	N CA	SER SER	345 345	19.107	3.888	49.067	1.00 25.65	BLGL
MOTA	2597	CB	SER.	345	20.754	5.061	49.530	1.00 25.43	BLGL
ATOM	2598	OG	SER	345	21.600	4.654	50.582	1.00 31.71	BLGL
ATOM	2599	С	SER	345	20.780	2.853	48.380	1.00 25.28	BLGL
ATOM	2600	0	SER		21.554	3.183	47.479	1.00 24.47	BLGL
ATOM	2601	N	GLY	346	20.662	1.604	48.823 48.220	1.00 24.37 1.00 21.46	BLGL BLGL
ATOM	2602	CA	GLY	346 346	21.414 20.430	0.518 -0.252	47.360	1.00 21.40	BLGL
ATOM ATOM	2603 2604	o O	<b>GLY</b>	346	19.286	0.183	47.216	1.00 20.32	BLGL
ATOM	2605	N	TRP	347	20.834	-1.385	46.795	1.00 18.57	BLGL
ATOM	2606	CA	TRP	347	19.915	-2.145	45.959	1.00 18.47	BLGL
ATOM	2607	CB.	TRP	347	20.677	-3.115	45.057	1.00 19.55	BLGL
MOTA	2608	CG	TRP	347	20.976	-4.426	45.700	1.00 24.39	BLGL
MOTA	2609		TRP	347	20.205	-5.626	45.576	1.00 26.03 1.00 27.34	BLGL BLGL
MOTA	2610		TRP	347	20.843 19.035	-6.616 -5.963	46.361 44.878	1.00 27.34	BLGL
MOTA MOTA	2611 2612		TRP TRP	347 347	22.023	-4.725	46.533	1.00 24.43	BLGL
ATOM	2613		TRP	347	21.950	-6.039	46.931	1.00 24.87	BLGL
ATOM	2614		TRP	347	20.344	-7.926	46.467	1.00 27.61	BLGL
ATOM	2615	CZ3	TRP	347	18.541	-7.268	44.982	1.00 26.42	BLGL
ATOM	2616		TRP	347	19.195	-8.229	45.770	1.00 25.85	BLGL
ATOM	2617	C	TRP	347	18.910	-2.916 -3.255	46.807 46.347	1.00 17.94 1.00 16.07	BLGL BLGL
ATOM	2618 2619	O N	TRP	347 348	17.820 19.296	-3.255	48.047	1.00 10.07	BLGL
ATOM ATOM	2620	CA	ALA ALA	348	18.444		48.984	1.00 21.94	BLGL
MOTA	2621	СВ	ALA		18.387	-5.394	48.607	1.00 20.51	BLGL
ATOM	2622	C	ALA		18.948	-3.767	50.422	1.00 24.22	BLGL
ATOM	2623	0	ALA	348	20.138	-3.549	50.659	1.00 25.24	BLGL
ATOM	2624	N	THR		18.030	-3.870	51.379	1.00 25.44	BLGL
ATOM	2625	CA	THR		18.378	-3.774	52.789	1.00 25.50 1.00 26.44	BLGL
ATOM	2626	CB	THR		17.509 16.167	-2.738 -3.228	53.553 53.679	1.00 25.28	BLGL
MOTA MOTA	2627 2628		THR THR		17.500	-1.400	52.823	1.00 24.16	BLGL
MOTA	2629	C	THR		18.102	-5.139	53.383	1.00 26.30	BLGL
MOTA	2630	ŏ	THR		17.382	-5.942	52.791	1.00 26.26	BLGL
MOTA	2631	N	SER		18.671	-5.403	54.551	1.00 27.06	BLGL
ATOM	2632	CA	SER		18.463	-6.685	55.208	1.00 26.38	BLGL
MOTA	2633	CB	SER		19.252	-6.738	56.514	1.00 23.71	BLGL BLGL
ATOM	2634	OG	SER		18.812	-5.726	57.400	1.00 21.01 1.00 26.83	BLGL
ATOM	2635 2636	C	SER		16.975 16.509	-6.911 -8.046	55.490 55.520	1.00 26.83	BLGL
ATOM ATOM	2636 2637	O N	SER TYR		16.225	-5.830			BLGL
ATOM	2638	CA	TYR		14.796	-5.946			BLGL
ATOM	2639	CB	TYR		14,208	-4.566		1.00 32.17	BLGL
						4	_		

Fig. 4 cont.

MOTA

MOTA

ATOM

MOTA

ATOM

ATOM

ATOM

ATOM

2698

2699

2700

2701

2702

2703

2704

2705

CG

CD

C

0

N

CA

OE1

GLU

GLU

GLU

GLU

GLU

ASP

ASP

OE2 GLU

358

358

358

358

358

358

359

359

#### 166/174 BLGL 1.00 33.63 -3.829 57.352 14.911 2640 CG TYR 351 MOTA 57.083 1.00 35.43 BLGL -2.951 15.961 CD1 TYR 351 2641 MOTA BLGL -2.279 58.114 1.00 35.75 16.623 2642 TYR 351 MOTA CE1 1.00 35.69 BLGL 58.677 14.539 -4.020TYR 351 2643 CD2 MOTA 1.00 36.21 BLGL -3.355 59.717 15.193 351 2644 CE2 TYR MOTA BLGL 16.231 -2.488 59.427 1.00 35.60 351 TYR ATOM 2645 CZ 1.00 36.59 BLGL -1.828 60.451 16.865 2646 OH TYR 351 ATOM BLGL 1.00 30.90 -6.626 54.836 14.012 351 ATOM 2647 С TYR -7.159 55.055 1.00 30.86 BLGL 12.921 2648 TYR 351 0 ATOM BLGL 1.00 30.77 14.572 -6.604 53.633 352 ALA MOTA 2649 N 52.476 1.00 31.75 BLGL -7.220 2650 CA ALA 352 13.936 ATOM BLGL 1.00 30.75 14.611 -6.74451.202 352 MOTA 2651 CB ALA BLGL 1.00 33.29 -8.745 52.545 352 13.989 2652 С ALA ATOM 1.00 33.71 BLGL 13.411 -9.434 51.700 2653 ALA 352 MOTA 0 1.00 33.30 BLGL 53.549 14.680 -9.273ALA 353 MOTA 2654 N .14.804 -10.718 BLGL 53.706 1.00 33.02 2655 353 MOTA CA ALA 1.00 34.24 BLGL 54.908 353 15.687 -11.033 2656 СВ ALA MOTA 13.449 -11.409 1.00 32.34 BLGL 53.856 2657 353 MOTA C ALA 1.00 30.15 BLGL 13.270 -12.545 53.422 353 2658 ALA ATOM 0 12.496 -10.716 1.00 33.65 BLGL 54.466 2659 354 MOTA N GLU 1.00 35.34 BLGL 11.176 -11.284 54.668 354 ATOM 2660 CA GLU 1.00 35.98 BLGL 55.578 10.345 -10.375 354 ATOM 2661 CB GLU 1.00 37.66 BLGL 9.744 -9.163 54.894 GLU 354 ATOM 2662 CG BLGL 1.00 40.92 -8.378 55.818 8.831 MOTA 2663 CD GLU 354 1.00 42.14 BLGL 8.010 -7.584 55.310 354 ATOM 2664 OE1 GLU 1.00 41.70 BLGL 8.935 -8.548 57.055 354 ATOM 2665 OE2 GLU 1.00 36.54 BLGL 10.457 -11.503 53.343 2666 GLU 354 MOTA C 1.00 36.40 BLGL 53.228 9.614 -12.416 354 MOTA 2667 0 GLU 1.00 36.32 BLGL 10.735 -10.673 52.345 2668 TYR 355 ATOM N BLGL 51.046 1.00 35.27 10.072 -10.778 MOTA 2669 ÇA TYR 355 1.00 32.38 BLGL -9.381 50.496 9.800 TYR 355 2670 MOTA CB BLGL -9.339 49.445 1.00 32.93 8.715 MOTA 2671 CG TYR 355 BLGL 48.087 1.00 31.94 9.022 -9.211CD1 TYR 355 ATOM 2672 1.00 30.60 BLGL 47.126 -9.141 8.014 2673 CE1 TYR 355 MOTA 1.00 31.34 BLGL 7.372 -9.403 49.812 CD2 TYR 2674 355 MOTA BLGL 1.00 31.48 48.864 355 6.364 -9.333 ATOM 2675 CE2 TYR BLGL 1.00 32.10 6.688 -9.198 47.524 355 MOTA 2676 CZ TYR 46.593 1.00 32.53 BLGL -9.084 5.679 355 MOTA 2677 OH TYR 1.00 36.46 BLGL 355 10.873 -11.590 50.034 MOTA 2678 C TYR 1.00 33.16 BLGL 10.306 -12.262 49.177 MOTA 2679 0 TYR 355 BLGL 50.133 1.00 39.53 12.196 -11.513 356 ATOM 2680 N ASP 1.00 42.86 BLGL 49.241 13.079 -12.251 2681 ASP 356 **ATOM** CA BLGL 48.096 1.00 43.64 13.568 -11.355 ATOM 2682 CB ASP 356 1.00 44.35 BLGL 47.182 14.568 -12.064 ASP 356 MOTA 2683 CG BLGL 15.202 -11.382 46.349 1.00 42.98 356 ATOM 2684 OD1 ASP 1.00 45.31 BLGL 47.293 14.715 -13.303 ATOM 2685 OD2 ASP 356 BLGL 50.045 1.00 45.45 14.278 -12.741 ATOM 2686 C ASP 356 BLGL 50.133 1.00 47.13 15.302 -12.058 2687 ASP 356 ATOM O BLGL 14.165 -13.931 50.650 1.00 46.19 ATOM 2688 N PRO 357 1.00 45.78 BLGL 50.688 12.983 -14.810 357 2689 CD PRO ATOM BLGL 51.447 1.00 46.80 15.260 -14.493 MOTA 2690 PRO 357 CA 1.00 46.98 BLGL 52.196 PRO 357 14.578 -15.627 CB MOTA 2691 BLGL 13.567 -16.109 51.196 1.00 46.25 2692 PRO 357 ATOM CG 1.00 48.11 BLGL 16.412 -14.990 50.581 357 PRO MOTA 2693 С BLGL 17.562 -15.006 1.00 48.32 51.007 MOTA 2694 O PRO 357 1.00 49.36 BLGL 16.075 -15.381 17.019 -15.911 49.358 358 ATOM 2695 N GLU 1.00 51.27 BLGL 48.385 ATOM 2696 CA GLU 358 1.00 53.72 BLGL 16.257 -16.304 47.125 GLU 358 2697 CB ATOM

Fig. 4 cont.

15.040 -17.170

15.414 -18.587 15.886 -19.331

15.244 -18.955

18.142 -14.958

19.319 -15.232

17.768 -13.850

18.717 -12.847

1.00 58.04

1.00 62.05

1.00 63.62

1.00 64.62

1.00 52.75

1.00 53.92

1.00 53.56

1.00 53.46

47.389

47.774

46.886

48.961

47.995

48.240

47.366

46.902

BLGL

BLGL

BLGL

BLGL

BLGL

BLGL

BLGL

BLGL

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ATOM	2706	СВ	ASP	359	18.203 -	12.213	45.609	1.00 56.56	BLGL
ATOM	2707	CG	ASP	359	18.748 -	12.887	44.366	1.00 58.60	BLGL
MOTA	2708		ASP	359	18.654 -		44.268	1.00 60.63	BLGL
MOTA	2709		ASP	359	19.268 -		43.485	1.00 59.51 1.00 51.60	BLGL BLGL
MOTA	2710	C	ASP	359	18.959 19.876		47.928 48.742	1.00 50.90	BLGL
ATOM	2711	0	ASP	359 360	18.132 -		47.865	1.00 51.06	BLGL
ATOM .		N	ALA ALA	360	18.226	-9.578	48.768	1.00 50.62	BLGL
MOTA MOTA	2713 2714	CA CB	ALA	·360	16.945	-8.767	48.697	1.00 49.16	BLGL
ATOM	2715	C	ALA	360	18.471 -		50.193	1.00 50.90	BLGL
ATOM	2716	ō	ALA	360	19.164	-9.403	50.973	1.00 49.67	BLGL
ATOM	2717	N	GLY	361	17.896 -		50.515	1.00 52.39	BLGL
MOTA	2718	CA	GLY	361	18.042 -		51.837	1.00 52.85	BLGL
MOTA	2719	C	GLY	361	19.481 -		52.312	1.00 53.39	BLGL BLGL
MOTA	2720	0	GLY	361	19.809 -		53.378	1.00 54.42 . 1.00 53.32	BLGL
ATOM	2721	N	LYS	362	20.351 - 21.737 -		51.540	1.00 53.32	BLGL
ATOM	2722 2723	CA CB	LYS LYS	362 362	22.081		52.329	1.00 57.86	BLGL
ATOM ATOM	2724	CG	LYS	362	21.401 -		51.495	1.00 59.76	BLGL.
ATOM	2725	CD	LYS	362	22.199 -		50.251	1.00 61.95	BLGL
ATOM	2726	ÇE	LYS	362	21.745 -		49.698	1.00 63.37	BLGL
ATOM	2727	NZ	LYS	362	22.557 -	-17.264	48.522	1.00 62.07	BLGL
ATOM	2728	С	LYS	362	22.741 -	-12.034	50.953	1.00 53.61	· BLGL
MOTA	2729	0	LYS	. 362	23.823 -		50.770	1.00 54.78	BLGL
ATOM .	2730	N	TRP	363	22.376		50.323	1.00 52.09	BLGL BLGL
ATOM	2731	CA	ŢRP	363	23.236		49.357 47.948	1.00 49.55 1.00 53.13	BLGL
ATOM	2732	CB	TRP	363 363	23.048 · 23.559 ·		47.792	1.00 58.47	BLGL
atom Atom	2733 2734	CG	TRP TRP	363	24.840		48.201	1.00 61.21	BLGL
MOTA	2735	CE2		363	24.867		47.894	1.00 62.60	$\mathtt{BLGL}$
ATOM	2736	CE3		363	25.966		48.802	1.00 63.42	BLGL
ATOM	2737		TRP	363	22.885	-13.277	47.262	1.00 60.70	BLGL
MOTA	2738	NE1	TRP	363	23.663		47.320	1.00 62.38	BLGL
ATOM	2739		TRP	363	25.981		48.168	1.00 63.65	BLGL
MOTA	2740		TRP	363	27.076		49.076	1.00 64.57	BLGL BLGL
MOTA	2741		TRP	363	27.071	-8.765	48.757 49.354	1.00 63.75 1.00 45.74	BLGL
ATOM	2742 2743	¢ o	TRP TRP	363 363	22.900 23.315	-8.031	48,460	1.00 46.95	BLGL
MOTA MOTA	2743	Ŋ	PHE	364	22,143	-8.333	50.357	1.00 40.08	BLGL
ATOM	2745	CA	PHE	364	21.748	-6.939	50.478	1.00 36.02	BLGL
ATOM	2746	CB	PHE	364	20.798	-6.763	51.664	1.00 35.97	BLGL
MOTA	2747	CG	PHE	364	21.393	-7.163	52.989	1.00 35.49	BLGL
MOTA	2748		PHE	. 364	22.170		53.723	1.00 34.51	BLGL
ATOM	2749		PHE	364	21.194	-8.448	53.493	1.00 34.67	BLGL BLGL
ATOM	2750		PHE	364	22.739	-6.637 -8.834	54.937 54.705	1.00 33.03 1.00 33.39	BLGL
MOTA	2751 2752	CEZ	PHE S	364 364	21.759 22.534	-7.927	55.429	1.00 33.77	Brer .
ATOM ATOM	2753	C	PHE	364	22.978	-6.061	50.655	1.00 33.99	BLGL
ATOM	2754	ŏ	PHE	364	23.998	÷6.506	51.181	1.00 34.27	BLGL
ATOM	2755	N	GLY	365	22.881	-4.816	50.208	1.00 30.67	BLGL
MOTA	2756	CA	GLY	365	24.008	-3.915	50.322	1.00 28.90	BLGL
ATOM	2757	С	GLY	365	23.806	-2.610	49.581	1.00 27.08	BLGL
MOTA	2758	0	GLY	365	22.708	-2.058	49.571	1.00 27.26	BLGL
ATOM	2759	N	GLY	366	24.863	-2.122	48.943	1.00 26.06 1.00 22.87	BLGL BLGL
MOTA	2760	CA	GLY	366	24.777 24.434	-0.860 -0.934	48.230 46.757	1.00 22.45	BLGL
ATOM	2761 2762	CO	GLY GLY	366 366	23.680	-1.800	46.737	1.00 20.99	BLGL
ATOM ATOM	2763	Ŋ	SER		24.996	0.004	46.002	1.00 22.77	BLGL
ATOM	2764	CA	SER		24.779	0.098	44.566	1.00 21.36	BLGL
ATOM	2765	СВ	SER		25.081	1.511	44.079	1.00 19.13	BLGL
ATOM	2766	OG	SER		25.081	1.539	42.665	1.00 20.78	BLGL
ATOM	2767	С	SER		25.649	-0.877	43.802	1.00 20.92	BLGL
ATOM	2768	0	SER		26.828	-1.040	44.111	1.00 22.00	BLGL
MOTA	2769	N	ALA		25.072	-1.518	42.794	1.00 19.58	BLGL
MOTA	2770	CA	ALA		25.823	~2.474	41.992	1.00 19.49 1.00 18.00	BLGL BLGL
ATOM	2771	CB	ALA	368	25.069	-3.792	41.921	T.00 TO.00	עטאנט

Fig. 4 cont.

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					00 000	-1.928	40.595	1.00 19.35	BLGL
ATOM	2772	С	ALA	368	26.058				
ATOM	2773	0	ALA	368	26.610	-2.612	39.735	1.00 19.98	BLGL
ATOM	2774	N	VAL	369	25.656	-0.679	40.387	1.00 19.26	BLGL
ATOM	2775		VAL	369	25.775	-0.041	39.080	1.00 19.71	BLGL
ATOM	2776		VAL	369	24.391	0.041	38.379	1.00 16.72	BLGL
		-		369	23.863	-1.349	38.093	1.00 13.08	BLGL
MOTA	2777	CG1				0.804	39.265	1.00 10.69	BLGL
MOTA	2778	CG2		369	23.411				BLGL
ATOM	2779	С	VAL	369	26.357	1.366	39.124	1.00 20.80	
MOTA	2780	Q	VAL	369	26.139	2.156	38.201	1.00 21.48	BLGL
MOTA	2781	N	ASP	370	27.083	1.693	40.187	1.00 21.01	BLGL
ATOM	2782	CA	ASP	370	27.680	3.024	40.269	1.00 21.96	BLGL
ATOM	2783	СВ	ASP	370	28.401	3.226	41.617	1.00 20.78	BLGL
				370	29.224	2.016	42.042	1.00 26.31	BLGL
MOTA	2784	CG	ASP			1.027	42.529	1.00 27.68	BLGL
MOTA	2785	OD1		370	28.640				BLGL
MOTA	2786	OD2	ASP	370	30.466	2.045	41.893	1.00 31.81	
ATOM	2787	С	ASP	370 .	28.649	3.264	39.098	1.00 21.03	BLGL
MOTA	2788	0	ASP	370	28.886	4.405	38.695	1.00 16.48	BLGL
ATOM	2789	N	ASN	371	29.188	2.181	38.542	1.00 20.75	BLGL
	2790	CA.		371	30.126	2.291	37.431	1.00 21.39	BLGL
MOTA					31.159	1.161	37.506	1.00 19.36	BLGL
MOTA	, 2791	CB	ASN	371			37.257	1.00 17.69	BLGL
MOTA	2792	CG	ASN	371	30.554	-0.202		1.00 17.05	BLGL
MOTA	2793	OD1		371	29.412	-0.471	37.631		
ATOM	2794	ND2.	ASN	371 .	31,329	-1.081	36.635	1.00 15.28	BLGL
ATOM	2795	С	ASN	371	29.435	2.298	36.062	1.00 22.85	BLGL
MOTA	2796	0	ASN	. 371 .	30.088	-2.203	35.018	1.00 21.45	$\mathtt{BLGL}$
ATOM	2797	N	GLN	372	28.109	2.405	36.074	1.00 21.57	BLGL
				372	27.355	2.458	34.837	1.00 21.91	BLGL
ATOM	2798	CA	GLN			1.248	34.702	1.00 19.34	BLGL
MOTA	2799	CB	GLN	372	26.432				BLGL
ATOM	2800	CG	GLN	372	27.186	-0.043	34.541	1.00 19.05	
ATOM	2801	CD	GLN	372	26.332	-1.154	33,981	1.00 18.53	BLGL
ATOM	2802	OE1	GLN	372	25.802	-1.043	32.881	1.00 16.76	BLGL
ATOM	2803		GLN	372	26.199	-2.240	34.732	1.00 19.99	BLGL
ATOM	2804	C	GLN	372	26.550	3.750	34.783	1.00 22.49	BLGL
				372	25.693	3.927	33.920	1.00 24.48	BLGL
MOTA	2805	0	GLN				35.705	1.00 21.34	BLGL
MOTA	2806	N	ALA	373	26.842	4.658			BLGL
MOTA	2807	CA	ALA	373	26.155	5.940	35.755	1.00 21.66	
ATOM	2808	CB	ALA	373	26.301	6.544	37.148	1.00 20.20	BLGL
MOTA	2809	C	ALA	373	26.702	6.914	34.705	1.00 22.35	BLGL
ATOM	2810	0	ALA	373	27.707	6.638	34.038	1.00 21.94	BLGL
ATOM	2811	N	LEU	374	26.025	8.048	34,555	1.00 21.60	BLGL
	2812	CA	LEU	374	26.454	9.080	33.617	1.00 21.79	BLGL
ATOM						9.548	32.763	1.00 19.88	BLGL
ATOM	2813	СВ	LEU	374	25.273			1.00 19.67	BLGL
ATOM	2814	CG	LEU	374	24.631	8.408	31.962		
ATOM	2815	CD1	LEU	374	23.430	8.928	31.196	1.00 19.92	BLGL
MOTA	2816	CD2	LEU	374	25.650	7.809	31.011	1.00 17.34	BLGL
MOTA	2817	С	LEU	374	27.040	10.236	34.431	1.00 22.87	BLGL
MOTA	2818	Ο.	LEU	374	27.314	11.319	33.905	1.00 21.82	BLGL
ATOM	2819	N	PHE	375	27.214	9.981	35.728	1.00 21.81	BLGL
	2820			375	27.800	10.937	36.664	1.00 23.69	BLGL
ATOM		CA	PHE			11.387	37.722	1.00 22.43	BLGL
ATOM	2821	CB	PHE	375	26.780				BLGL
ATOM		CG	PHE		25.641	12.195	37.169		
MOTA	2823	CD1	PHE	375	24.652				BLGL
ATOM	2824	CD2	PHE	375	25.563	13.566	37.407		BLGL
ATOM	2825	CE1	PHE	375	23.606	12.343	35.856	1.00 21.26	BLGL
ATOM	2826		PHE		24.521				BLGL
					23.543				BLGL
ATOM	2827	CZ	PHE				37.356		BLGL
ATOM	2828	C	PHE		28.928				BLGL
ATOM	2829	0	PHE		28.849				
ATOM	2830	N	ASP	376	29.975	10.890			BLGL
ATOM	2831	CA	ASP	376	31.070	10.217	38.449	1.00 24.64	BLGL
ATOM	2832	CB	ASP		32.369		38.382	1.00 25.91	BLGL
ATOM	2833	ÇG	ASP		32.243				BLGL
									BLGL
ATOM	2834		. ASP		31.528				BLGL
ATOM	2835		ASP		32.885				BLGL
MOTA	2836	C	ASP		30.698				
MOTA	2837	0	ASP	376	29.621	10.349	40.344	1.00 22.18	BLGL

Fig. 4 cont.

					16	9/174			
ATOM	2838	N	PHE	377	31.610	9.333	40.625	1.00 24.93	BLGL
ATOM	2839	-	PHE	377	31.421	9.000	42.030	1.00 26.87	BLGL
ATOM	2840	-	PHE	. 377	32.652	8.256	42.530	1.00 24.91	BLGL BLGL
MOTA	2841		PHE	377	32.915	6.967	41.811 41.837	1.00 26.64 1.00 27.20	BLGL
ATOM	2842	CD1		377 377	34.185 31.891	6.394 6.298	41.037	1.00 27.20	BLGL
MOTA	2843 2844	CD2 CE1	PHE	. 377	34.434	5.168	41.209	1.00 27.98	BLGL
MOTA MOTA	2845		PKE	377	32.127	5.073	40.511	1.00 27.70	BLGL
ATOM	2846	CZ	PHE	377	33.402	4.505	40.546	1.00 28.28	BLGL
ATOM	2847	С	PHE	377	31.162	10.214	42.919	1.00 28.76	BLGL
MOTA	2848	0	PHE	377	30.660	10.084	44.041	1.00 29.47	BLGL BLGL
MOTA	2849	N	LYS	378 -	31.500	11.393	42.410 43.155	1.00 30.92 1.00 32.99	BLGL
ATOM	2850	CA	LYS	378 378	31.322 32.533	12.634 13.546	42.927	1.00 36.98	BLGL
ATOM .	2851 2852	CB CG	LYS	378 378	33.889	12.924	43.274	1.00 39.50	BLGL
ATOM	· 2853	CD	LYS	378	34.230	13.053	44.759	1.00 43.64	BLGL
ATOM	2854	CE	LYS	378	33.249	12.300	45.651	1.00 45.28	BLGL
ATOM	2855	NZ	LYS.	. 378	33.467	12.607	47.092	1.00 46.72	BLGL
ATOM	2856	С	LYS	378	30.040	13.391	42.800	1.00 32.50	BLGL
MOTA	2857	0	LYS	378	. 29.803	14.487	43.309	1.00 31.66 1.00 32.04	BLGL BLGL
MOTA	2858	N	GLY	379	29.224	12.816	41.919 41.544	1.00 32.04	BLGL
ATOM	2859	CA	GLY	379 379	27.975 - 28.092	13.453 14.430	40.397	1.00 32.10	BLGL
ATOM ATOM	·2860 2861	C	GLY GLY	379	27.146	15.159	40.085	1.00 32.60	BLGL
ATOM	2862	И	ARG	380	29.261	14.451	39.771	1.00 35.05	BLGL
ATOM	2863	CA	ARG	380	29.507	15.342	38.647	1.00 35.69	BLGL
ATOM	2864	CB	ARG	380	30.958	15.817	38.660	1.00 40.31	BLGL
ATOM	2865	CG	ARG	380	31.123	17.323	.38.592	1.00 48.35	BLGL
MOTA	2866	CD	ARG	380	32.569	17.728	38.876	1.00 55.04 1.00 61.15	BLGL BLGL
ATOM	2867	NE	ARG	380	33.058 33.782	17.213 16.100	40.164 40.318	1.00 61.13	BLGL
ATOM	2868 2869	CZ	ARG ARG	380 380	34.117	15.362	39.267	1.00 62.74	BLGL
MOTA MOTA	2870		ARG	380	34.178	15.720	41.529	1.00 60.75	BLGL
ATOM	2871	C	ARG	380	29.216	14.587	37.354	1.00 34.09	BLGL
ATOM	2872	0	ARG	380	29.551	13.404	37.213	1.00 34.62	BLGL
MOTA	2873	N	PRO	381	28.590	15.265	36.386	1.00 30.20	BLGL
MOTA	2874	CD	PRO	381	28.201	16.683	36.407	1.00 27.18 1.00 28.29	BLGL BLGL
ATOM	2875	CA	PRO	381	28.250 27.395	14.653 15.723	35.101 34.438	1.00 28.29	BLGL
ATOM ATOM	2876 2877	CB CG	PRO PRO	381 381	28.018	16.980	34.941	1.00 26.31	BLGL
ATOM	2878	C	PRO	381	29.453	14.278	34.260	1.00 26.53	BLGL
ATOM	2879	ō	PRO	381	30.436	15.014	34.221	1.00 27.34	BLGL
ATOM	2880	N	LEU	382	29.370	13.122	33.601	1.00 26.02	BLGL
ATOM	2881	CA	LEU	382	30.439	12.645	32.721	1.00 24.03	BLGL
ATOM	2882	CB	LEU	382	30.475	11.116	32.656	1.00 21.52 1.00 22.08	BLGL BLGL
MOTA	2883	CG	LEU	382 382	30.769 30.549	10.338 8.867	33.934 33.678	1.00 22.08	BLGL
ATOM ATOM	2884 2885		LEU	382 382	32.190	10.608	34.390	1.00 21.32	BLGL
MOTA	2886	C	LEU	382	30.128	13.174	31.336	1.00 23.10	BLGL
MOTA	2887	ŏ	LEU	382	28.964	13.412	30.996	1.00 22.81	BLGL
ATOM	2888	N	PRO	383	31160	13.364	30.511	1.00 22.83	BLGL
MOTA	2889	ÇD	PRO		32.593	13.134	30.744	1.00 21.59	BLGL
MOTA	2890	CA	PRO		30.919	13.873	29.159	1.00 22.58 1.00 22.02	BLGL BLGL
ATOM	2891	CB	PRO		32.327 33.101	13.950 12.953	28.559 29.345	1.00 22.02	BLGL
ATOM ATOM	2892 2893	CG	PRO PRO		29.959	13.00B	28.340	1.00 22.29	BLGL
ATOM	2894	Ö	PRO		29.346	13.491	27.395	1.00 23.29	BLGL
ATOM	2895	И	SER		29.815	11.739	28.718	1.00 23.07	BLGL
ATOM	2896	CA	SER		28.918	10.830	28.014	1.00 23.32	BLGL
ATOM	2897	CB	SER	384	29.189	9.387	28.438	1.00 23.43	BLGL
ATOM	2898	OG	SER		28.997	9.221	29.827	1.00 22.72	BLGL
ATOM	2899	C	SER		27.441	11.166		1.00 24.76	BLGL BLGL
ATOM	2900	0	SER		26.556	10.584	27.629 29.160		BLGL
ATOM	2901	N	LEU		27.166 25.792	12.094 12.474			BLGL
ATOM ATOM	2902 2903	CA CB	LEU		25.721	13.380			BLGL
FILOU	200	ÇD	220	555					

Fig. 4 cont.

					17	0/174			
ATOM	2904	CG	LEU	385	24.332	13.873	31.055	1.00 23.33	BLGL
ATOM	2905	CD1		385	23.424	12.687	31.367	1.00 22.86	BLGL
MOTA	2906	CD2		385	24.458	14.778	32.268	1.00 20.09	BLGL
MOTA	2907	С	LEU	385	25.250	13.207	28.193	1.00 26.26	BLGL BLGL
MOTA	2908	0	LEU.	385	24.041	13.255 13.763	27.958 27.404	1.00 25.15 1.00 28.46	BLGL
MOTA	2909	N	HIS HIS	386 . 386	26.161 25.789	14.512	26.213	1.00 32.60	BLGL
ATOM ATOM	2910 2911	CA CB	HIS	386	26.937	15.437	25.816	1.00 37.77	BLGL
MOTA	2912	CG	HIS	386	27.172	16.539	26.799	1.00 45.65	BLGL
ATOM	2913	CD2		386	26.393	17.016	27.801	1.00 45.94	BLGL
MOTA	2914	NDI	HIS	3 <b>8</b> 6.	28.330	17.291	26.820	1.00 48.26	BLGL
MOTA	2915	CE1		386	28.254	18.180	27.795	1.00 49.16	BLGL
ATOM	2916	NE2		386	27.089	18.033	28.405 25.025	1.00 49.07 1.00 32.02	BLGL BLGL
MOTA	2917	C	HIS	·- 386 386	25.392 25.011	13.656 14.184	23.023	1.00 34.90	BLGL
ATOM ATOM	2918 2919	O N	VÁL	387	25.467	12.341	25.177	1.00 29.53	BLGL
MOTA	2920 •		VAL	387	25.117	11.461	24.075	1.00 27.58	BLGL
ATOM	2921	CB	VAL	387	. 25.236	9.974	24.496	1.00 27.23	BLGL
ATOM	2922	CG1	VAL	387	24:191	9.637	25.547	1.00 25.13	BLGL
MOTA	2923		VAL	387	25.114	9.072	23.276	1.00 23.77	BLGL
MOTA	2924	C	VAL	387	23.701	11.760	23.572	1.00 26.94 1.00 26.81	BLGL BLGL
MOTA	2925	0	VAL	387 388 ·	23.450 22.78B	11.750 12.060	22.369 24.491	1.00 25.61	BLGL
ATOM ·	·2926 2927	N .	PHE	388 · 388	21.403	12.339	24.136	1.00 26.79	BLGL
ATOM	2928	CB	PHE	388	20.586	12.619		1.00 25.81	· BLGL
ATOM		. CG	PHE	388	20.433	11.432	26.272	1.00 26.19	BLGL
ATOM	2930		PHE	388	21.003	11.412		1.00 27.32	BLGL
MOTA	2931		PHE	388	19.728	10.317	25.834	1.00 25.78	- BLGL
MOTA	2932		PHE	388	20.873	10.300	28.355	1.00 27.00 1.00 26.04	BLGL BLGL
ATOM	2933		PHE	388 388	19.592 20.166	9.198 9.189	26.647 27.909	1.00 26.12	BLGL
ATOM ATOM	2934 2935	CZ C	PHE PHE	388	21.188	13.470		1.00 29.70	BLGL
ATOM	2936	ō	PHE	388	20.176	13.496	22.424	1.00 29.14	BLGL
MOTA	2937	N	GLN	389	22.125	14.412	23.102	1.00 31.10	BLGL
ATOM	2938	CA	GLN	389	22.022	15.532	22.174	1.00 32.46	BLGL
MOTA	2939	CB	GLN	389	22.603	16.797	22.793	1.00 35.41	BLGL BLGL
ATOM	2940	CG	GLN	389	22.086 22.807	17.088 18.261	·24.177 24.818	1.00 44.69 1.00 50.70	BLGL
ATOM ATOM	2941 2942	CD OF 1	GLN GLN	389 389	22.674	19.401	24.372	1.00 52.70	BLGL
MOTA	2943		GLN	389	23.588	17.985	25.866	1.00 53.54	BLGL
ATOM	2944	С	GLN	389	22.779	15.221	20.893	1.00 30.30	· BLGL
MOTA	2945	0	GLN	389	22.270	15.416	19.790	1.00 31.42	· BLGL
ATOM	2946	N	TYR	390	23.993	14.715	21.051	1.00 28.80	BLGL
ATOM	2947	CA	TYR	390	24.851	14.403	19.917	1.00 30.88	BLGL BLGL
ATOM	2948	CB	TYR TYR	390 390	26.204 26.963	13.911 14.956	20.427 21.217	1.00 35.50 1.00 41.72	BLGL
ATOM ATOM	2949 2950	CG CD1		390	28.151	14.632	21.871	1.00 45.09	BLGL
MOTA	2951		TYR	390	28.861	15.595	22.603	1.00 47.24	BLGL
ATOM	2952		TYR	390	26.496	16.273	21.313	1.00 42.36	BLGL
ATOM	2953	CE2	TYR	390	27.192	17.240	22.043		BLGL
ATOM	2954	CZ	TYR		28.376	16.894	22.686		BLGL
ATOM	2955	ОН	TYR		29.078	17.841	23.406		BLGL BLGL
ATOM	2956	C	TYR		24.298 24.591	13.425 13.553	18.889 17.704		BLGL
ATOM ATOM	2957 2958	0 N	TYR VAL		23.508	12.450	19.324	1.00 27.33	BLGL
ATOM	2959	CA	VAL		22.943	11.488	18.381		BLGL
ATOM	2960	CB	VAL		22.008	10.476	19.087	1.00 23.42	BLGL
ATOM	2961		VAL	391	22.803	9.635	20.061		BLGL
ATOM	2962		VAL		20.886	11.202	19.805		BLGL
MOTA	2963	C	VAL		22.154	12.226			BLGL BLGL
ATOM	2964	0	VAL		22.028	11.749 13.400	16.175 17.647		BLGL
ATOM ATOM	2965 2966	N CA	ASP ASP		21.635 20.862	14.200			BLGL
ATOM	2967	CB	ASP		20.002	15.323			BLGL
ATOM	2968	CG	ASP		18.986	14.820		1.00 34.68	BLGL
ATOM	2969		ASP		18.444	15.617			BLGL

Fig. 4 cont.

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ATOM	2970	OD2	ASP	392	18.618	13.636	18.167	1.00 3	5.22	BLGL
ATOM	2971	С	ASP	392	21.731	14.818	15.621	1.00 3	3.35	BLGL
ATOM	2972	0	ASP	392	21.467	14.650	14.430	1.00 3	15.61	BLGL
ATOM	2973	N	THR	393	22.777	15.526	16.035	1.00 3	4.96	BLGL
ATOM	2974	CA	THR	393	23.664	16.215	15.105	1.00 3	34.87	BLGL
ATOM	2975	CB	THR	393	23.998	17,626	15.602	1.00 3	35.87	BLGL
ATOM	2976	OG1	THR	393	24.820	17.526	16.774		37.14	BLGL
MOTA	2977	CG2	THR	393	22.726	18.392	15.952	1.00 3	35.93	BLGL
ATOM	2978	С	THR	393	24.991	15.518	14.908	1.00 3	36.53	BLGL
MOTA	2979	0	THR	393	25.462	15.358	13.787	1.00 3	36.72	BLGL
MOTA	2980	N	GLY	394	25.596	15.115	16.014		38.00	BLGL
ATOM	2981	CA	GLY	.394	26.896	14.481	15.961	1.00 3		BLGL
ATOM	2982	С	GLY	394	27.828	15.442	16.679	1.00 4	10.97	BLGL
ATOM	2983	0	GLY	394	27.389	16.494	17.143	1.00 4	10.87	BLGL
ATOM	2984	N	THR	<b>3</b> 95	29.105	15.107	16.787	1.00 4		BLGL
ATOM	2985	CA	THR	395	30.043	15.990	17.461	1.00 4	15.02	BLGL
MOTA	2986	CB	THR	. 395	30.967	15.197	18.393	1.00 4	13.84	BLGL.
MOTA	2987	OG1	THR	395	31.206	13,896	17.840	1.00 4		BLGL
ATOM	2988	CG2	THR	395	30.340	15.054	19.753	1.00		BLGL
ATOM	. 2989	С	THR	395	30.883	16.752	16.443	1.00	18.88	$\mathtt{BLGL}$
ATOM	2990	0	THR	395	31.470	16.155	15.536	1.00	-	BLGL
ATOM	2991	N	PRO	396	30.941	18.089	16.578	1.00		BLGL
ATOM	2992	CD	PRO	396	30.225	18.889	17.594	1.00		BLGL
MOTA	2993	CA	PRO	396	31.712	18.955	15.672	1.00		BLGL
MOTA	2994	CB	PRO	396	31.537	20.343	16.291	1.00		BLGL
ATOM	2995	CG	PRO	396	30.173	20.256	16.948		52.73	
ATOM	2996	С	PRO	396	33.188	18.543	15.578	1.00		BLGL
' ATOM	2997	O	PRO	396	33.678	18.369	14.436	1.00	54.55	BLGL
END										



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# PVS

		9	19	29	39		
		-ATTYRGVDW	SSVVVEERAG	VSYKNTNGNA	<b>QPLENILAAN</b>	39	MT
		-ATOAKCADM	SSVMVEERAG	VRYKNVNGOE	KPLEYILAEN	39	HI
		- ALMABANDI	SSILLLEDEG	YSYKNI.NGOT	OALETILADA	39	AA
	GLYVEKVSGL	-WDIIKONDI	CCTINIEECC	AVEANESCER	ODIENTLKEA		BL
				50	60	00	
10	20	30	40	30	00		
49	54	61	71	81	91		
GVNTVRQRVW	VNPAD	GNYNLDY	NIAIAKRAKA	AGLGVYIDFH	YSDTWADPAH	91	
GVNMVRORVW	VNPWD	GNYNLDY	NIQLARRAKA	AGLGLYINFH	YSDTWADPAH	91	
GINSTRORVW	VNPSD	GSYDLDY	NLELAKRVKA	AGMSLYLDLH	LSDTWADPSD	91	
CUNVURURTW	NDPYDANGNG	VECCUNDIFIC	ATOTGKRANA	NGMKLLADFH	YSDFWADPAK"	120	
70.	80	90	100	110	120		
70,	00	70	100	220			
7.00		120	130	140	. 150		
. 100	1.10					150	
QTMPAGWP-S	DIDNLSWKLY	NYTLDAANKL	QNAGIQPTIV	SIGNEIRAGE	TWPIGRIENW	150	
QTTPAGWP-S	DINNLAWKLY	NYTLDSMNRF	ADAGIQVDIV	SIGNETTOGL	LWPLGKINNW		
QTTPSGWSTT	DLGTLKWQLY	NYTLEVCNTF	AENDIDIEII	SIGNEIRAGL	LWPLGETSSY	151	
QKAPKAWANL	NEEDKKTALY	QYTKQSLKAM	KAAGIDIGMV	QVGNETNGGL	AGETDW	176	•
130	140	150	· 160	170	1.76		
160	170	180	190	200	<u> </u>		
	AWGIKDSSLS			WYTNVIKOGT	LELSDFDMMG	210	1
ANTARILION	AWGVKDSRLN	DEDETMUNT	MCMMMDAOMM	WYTWULSOCP	FEMSDEDMMG	210	}
INTARPPHOA	AWGVKDSNLA	LULUINATIO	DCFICFIOOONA MGMMD1ÖMM	CALANTOR	LLSTOFOVEG	211	
SNIGALLHSG	AWGVKDSNLA	TTPKIMIHLD	DGWSWDQQNI	TADELUBII	THREADING	230	
	SQAVRETD			TAETLINKH	230	250	•
186		204	214		230		
					265		
220	230	240	250	255	265		
VSFYPFYSSS	ATLSALKSSL	DNMAKTWNKE	IAVVETNWPI	SCPNP	RYSFPSDVKN	265	
VSFYPFYSAS	ATLDSLRRSL	NNMVSRWGKE	VAVVETNWPT	SCPYP	RYQFPADVRN	265	5
VSYYPFYSAS	ATLASLKTSL	ANLOSTYDKP	VVVVETNWPV	SCPNP	AYAFPSDLSS	266	5
SSYYPFWH	GTLKNLTSVL	TSVADTYGKK	VMVAETSYTY	TAEDGDGHGN	TAPKNGQTLN	288	3
238	248	258	268		. 288		
250	240	250	200	<b></b>			
275	285	. 294					
	FITNVANIVS		VEIDDANEU			30;	2
IPFSPEGQTT	ETTNVANIVS	SVS-KGVGLE	IWEPAWIN			302	_
VPFSAAGQTQ	<b>2VVNAVZQIY</b>	SVS-KGVGLE	AME SAMTH				
I PFSVAGQQE	FLEKLAAVVE	ATT-DGLGVY	YWEPAWIG			30:	_
NPVTVQGQAN	AVRDVIQAVS	DVGEAGIGVE			LWETYGSGWA	348	3
298	308	318	328	338	348		
	309	318	328				
	NANLGSS		SGOALSSLSV	FORI	332		
	NANI.CSS	CADMTMET D-	SCOALSSISV	FHRI	332		
	NAGLGSS	CYDNI WADAM	ADENAEGIEM CONTROL	TERL			
	NAGLGSS	CHDMDMADII	TOUVIESTEL	<b>たしくハンル</b> でからた TOETA	KN 399		
	DAGKWEGGSA						
358	368	377	387	397			



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## PVS

		. 9	19	. 29	39		
			SSVVVEERAG	VSYKNTNGNA	QPLENILAAN	39	MT
		-ALOYKGVDW	SSVMVEERAG	VRYKNVNGQE	KPLEYILAEN	39	HI
		-ALTYRGADT	SSLLLLEDEG	YSYKNLNGOT	QALETILADA	39	AA
AUDDSCTAKS	GLYVEKVSGL	RKDFIKGVDV	SSITALEESG	VAFYNESGKK	QDIFNTLKEA	60	BL
ARRESCIANS		-ALTYRGADI	SSLLIEEDAG	ISYKNLNGET	QALEDILVNN	39	ΑT
	M	NKDFTKGADV	SSVIALENSG	VTFYNTNGKR	QDIFTTLKQA	41	BS
	NTGVAD	NTPFYVGADI	SYVNEMESCG	ATYRD-OGKK	VDPFQLFADK	45	PF
	. 6	16		35	45.		
•			_•	•			
49	54	61	71	81	91	-	
CUNTURORUW	VNPAD		NIAIAKRAKA	AGLGVYIDFH	YSDTWADPAH	91	
GVNMVRORVW	VNPWD	GNYNLDY	NIOLARRAKA	AGLGLYINFH	YSDTWADPAH	91	
GTNSTRORVW	VNPSD	GSYDLDY	NLELAKRVKA	AGMSLYLDLH	LSDTWADPSD	91	
GVNYVRVRIW	NDPYDANGNG	YGGGNNDLEK	AIQIGKRANA	NGMKLLADFH	YSDFWADPAK	120	
GVNSIRORVW	VDPSD	GSYDLDY	NLKLAKRVQA	.AGMSIYLDLH	LSDTWADPSD	91	
GVNYVRVRIW	NHPYDSNGNG	YGGGNNDVQK	AIEIGKRATA	NGMKVLADFH	YSDFWADPAK	101	
GADLVRVRLW	HNATWT	KYSDLKD	VSKTLKRAKN	AGMKTLLDFH	YSDTWTDPEK	98	
55	61	68	78	88	98		
,							
99	109		129	139	145		
OTMPAGWP	SDIDNLSWKL	YNYTLDAANK	LQNAGIQPTI	VSIGNEIRAG	LLWPTG	145	
OTTPACWP	SDINNLAWKL	YNYTLDSMNR	FADAGIQVDI	VSIGNEITQG	LLWPLG	145	
OTTPSGWST-	TDLGTLKWOL	YNYTLEVCNT	FAENDIDIEI	ISIGNEIRAG	LLWPLG	146	i
OKAPKAWAN-	LNFEDKKTAL	YOYTKQSLKA	MKAAGIDIGM	VQVGNETNGG	LA	171	
OTTPTGWST-	TDIDTLTWOL	YNYTLEVCNT	FAENDIDVEI	VSIGNEISSG	LLWPLG	146	
OKVPKAWAN-	LSFEAKKAKL	YEYTKQSLQK	MIKEGVDIGM	VQVGNETTGG	FA	152	
QFIPKAWAHI	TDTKELAKAL	YDYTTDTLAS	LDQQQLLPNL	VQVGNETNIE	ILQAEDTLVH	158	3
109	118	128	138	148	158		
155	165	175	185	195			
RTENWANIAR	LLHSAAWGIK	DSSLSPKPKI	MIHLDNGWDW	GTQNWWYTNV	LKQGTLELSD	205	
KTNNWYNIAR	LLHSAAWGVK	DSRLNPKPKI	MAHTDNGMNM	DTQNWWYTNV	LSQGPFEMSD	205	
ETSSYSNIGA	LLHSGAWGVK	DSNLATTPKI	MIHLDDGWSW	DQQNYFYETV	LATGELLSTD	206	
GETDWAKMSQ	LFNAGSQAVR	ETDSNILV	ALHFTNPETS	GRYAWIAETL	HRHHVD	225	
KTSNYDNIAK	LLHSGAWGVK	DSDLTTTPKI	MIHLDNGWDW	DEQEYFYKTV	LATGSLLSTD	206	
GETDWTKMCQ	LFNEGSRAVR	ETNSNILV	ALHFTNPETA	GRYSFIAETL	SKNKVD	206	
GI PNWQRNA <b>T</b>					ENGVID	214	3
168	178	188	198	208	214		
	_	•		e==	0.60		
215		235			260	261	
FDMMGVSFYP	FYSSSATLSA	LKSSLDNMAK	TWNKEIAVVE	TNWPISC	PNPRYSFP	260 260	-
FDMMGVSFYP	FYSASATLDS	LRRSLNNMVS	RWGKEVAVVE	TNWPTSC	PYPRYQFP		_
FDYFGVSYYP	FYSASATLAS	LKTSLANLQS	TYDKPVVVVE	TNWPVSC	PNPAYAFP		
YDVFASSYYP	FWHGTLKN	LTSVLTSVAD	TYGKKVMVAE	TSYTYTAEDG	DGHGNTAPKN		
FDLMGVSYYP	FYSSEATLSS	LKTSLTNMQS	NADKBAAAAE	TNWPVSC	PDPEYSFP		
YDVFASSYYP	FWHGTLQN	LTSVLKAVAN	TYGKKVMVAE	TSYTYTALD	DGHGNTAPKS	-	
					DQAGNVLGEK	27.	,
224	233	243	253	263	213		
070	300	200	200				
270	280	289	299			30:	2
SDVKNIPESP	FEGULLETINA	WALASSAZ-K	CACT CAME DE	WILL		30	
ADVKNVPESA	AGOTOXIOSV	ANVVSSVS-K	. GVGLEIWEPA	/ MIC			
SULSSIPESV	AGQQEFTEKL	AAVVEATT-D	CTCUEVEEP	MIG	EKNKALWETY	33	
GQTLNNPVTV	A COEFFE FOR	TOWASDAGEN	CICIVVMEDA	MID		30	
SULTSIFFSA	. AGUEEF LEKL	- MEVVEGVI-L - MEVVEGVI-L	CTCVEVMEDA	MIDNCDKTO	EKNKVLWETY		
GUILFIFISV	OGOTANT AND	TILAVANIGKA	. GLGVEIWE <i>lf</i> . CMCVIVWED?	MACABLD			
			311 - GMGVIIWE <i>PF</i>			. J.	-
283	293	301	211				

Fig. 6





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			174/174		PVS	
		314	322	332		
	NA	NLGSSCADNT	MFSQSGQA	LSSLSVFQRI		332
	NA	NLGSSCADNT	MFTPSGQA	LSSLSVFHRI		332
	NA	GLGSSCADNL	MVDYT-TDEV	YESIETLGEL		334
GSGWATSYAA	EYDPEDAGKW	FGGSAVDNQA	LFDFKGRP	LPSLHVFQYV	DTGTPFKN	399
	NA	GLGSSCADNL	MVDVN-TDEV	LESVTVFEDL		334
GSGWASSYAA	EYDPEDAGKW	YGGSAVDNQA	LFDFNGHP	LPSLQVFQYA		372
	TLW	GKGSHWENAS	FEDATRKNNA	LPAFLFFKAD	YQASAQAE	359
	321	331	341	351		

Fig. 6 cont.

Modtaget 0 8 APR. 2003 PVS

# 10319.000.ST25.txt SEQUENCE LISTING.

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 The His Leu Asp 180
 Asn Gly Trp Asp 1319.000.ST25.txt
 Trp Tyr Tyr 190

 Thr Asn Val 195
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 Met 210
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 Ala Leu Lys Ser Ser Leu Asp Asn Met Ala Lys Thr Trp Asn Lys Glu 240

 Tle Ala Val Val 245
 Thr Asn Trp Pro 125
 Ser Cys Pro Asn Pro Arg

 Tyr Ser Phe Phe Pro Ser Asp Val Lys Asn Ile Pro Phe Ser Pro Glu Gly 270
 Glu Gly Ala Asn Ile Val 285
 Ser Val Ser

 Arg 290
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Glu Tyr Ile Leu Ala Glu Asn Gly Val Asn Met Val Arg Gln Arg Val

Trp Val Asn Pro Trp Asp Gly Asn Tyr Asn Leu Asp Tyr Asn Ile Gln 50 60

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Lys Lys Gln Asp Ile Phe Asn Thr Leu Lys Glu Ala Gly Val Asn Tyr 50 60

Val Arg Val Arg Ile Trp Asn Asp Pro Tyr Asp Ala Asn Gly Asn Gly 65 70 75

Tyr Gly Gly Asn Asn Asp Leu Glu Lys Ala Ile Gln Ile Gly Lys 85 90 95

Arg Ala Asn Ala Asn Gly Met Lys Leu Leu Ala Asp Phe His Tyr Ser

Asp Phe Trp Ala Asp Pro Ala Lys Gln Lys Ala Pro Lys Ala Trp Ala 115 120 125 Asn Leu Asn Phe Glu Asp Lys Lys Thr Ala Leu Tyr Gln Tyr Thr Lys 130 135 140 Gln Ser Leu Lys Ala Met Lys Ala Ala Gly Ile Asp Ile Gly Met Val 145 150 160 Gln Val Gly Asn Glu Thr Asn Gly Gly Leu Ala Gly Glu Thr Asp Trp 165 170 175 Ala Lys Met Ser Gln Leu Phe Asn Ala Gly Ser Gln Ala Val Arg Glu 180 185 190 Thr Asp Ser Asn Ile Leu Val Ala Leu His Phe Thr Asn Pro Glu Thr 195 200 205 Ser Gly Arg Tyr Ala Trp Ile Ala Glu Thr Leu His Arg His His Val 210 215 220 Asp Tyr Asp Val Phe Ala Ser Ser Tyr Tyr Pro Phe Trp His Gly Thr 225 230 235 240 Leu Lys Asn Leu Thr Ser Val Leu Thr Ser Val Ala Asp Thr Tyr Gly 245 250 255 Lys Lys Val Met Val Ala Glu Thr Ser Tyr Thr Tyr Thr Ala Glu Asp 260 265 270 Gly Asp Gly His Gly Asn Thr Ala Pro Lys Asn Gly Gln Thr Leu Asn 275 280 285 Asn Pro Val Thr Val Gln Gly Gln Ala Asn Ala Val Arg Asp Val Ile 290 295 300 Gln Ala Val Ser Asp Val Gly Glu Ala Gly Ile Gly Val Phe Tyr Trp 305 310 315 320 Glu Pro Ala Trp Ile Pro Val Gly Pro Ala His Arg Leu Glu Lys Asn 325 330 335 Lys Ala Leu Trp Glu Thr Tyr Gly Ser Gly Trp Ala Thr Ser Tyr Ala 340 345 350 Ala Glu Tyr Asp Pro Glu Asp Ala Gly Lys Trp Phe Gly Gly Ser Ala 355 360 365 Val Asp Asn Gln Ala Leu Phe Asp Phe Lys Gly Arg Pro Leu Pro Ser 370 375 380

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 Trp Val Asp Pro Ser Asp Gly Ser Tyr Asp Leu Asp Tyr Asn Leu Lys 50 60
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10319.000.ST25.txt
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130 135 140 Asn Glu Thr Thr Gly Gly Phe Ala Gly Glu Thr Asp Trp Thr Lys Met 145 150 155 160 Cys Gln Leu Phe Asn Glu Gly Ser Arg Ala Val Arg Glu Thr Asn Ser 165 170 175 Asn Ile Leu Val Ala Leu His Phe Thr Asn Pro Glu Thr Ala Gly Arg 180 185 190 Tyr Ser Phe Ile Ala Glu Thr Leu Ser Lys Asn Lys Val Asp Tyr Asp 195 200 205 Val Phe Ala Ser Ser Tyr Tyr Pro Phe Trp His Gly Thr Leu Gln Asn 210 215 220 Leu Thr Ser Val Leu Lys Ala Val Ala Asn Thr Tyr Gly Lys Lys Val 225 230 235 240 Met Val Ala Glu Thr Ser Tyr Thr Tyr Thr Ala Glu Asp Gly Asp Gly 255

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Leu val Arg Val Arg Leu Trp His Asn Ala Thr Trp Thr Lys Tyr Ser 50 60

Asp Leu Lys Asp Val Ser Lys Thr Leu Lys Arg Ala Lys Asn Ala Gly 65 70 75

Met Lys Thr Leu Leu Asp Phe His Tyr Ser Asp Thr Trp Thr Asp Pro 85 90 95

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